

MedeA QSPR

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1 Key Benefits of MedeA QSPR

- Determination of geometric descriptors for organic molecules
- Evaluation of thermodynamic properties (of organic compounds) based on Group contributions
- Rapid property calculation enabling screening of compounds and/or providing input conditions for molecular simulations
- Provides thermophysical properties (based on Joback's Group Contribution method)
- Uses group contributions to compute properties based on correlations

2 Introduction

"MedeA QSPR: Property Prediction using Group Contributions" employs correlations to predict thermophysical properties, based on the chemical groups that constitute an organic molecule. The number and type of groups, and their contribution to each property, have been developed and described by Joback and Reid [1]. Only structural information of a chemical compound (a molecule) is used to calculate thermophysical and transport properties, by adding group parameters. This method uses a single group list for all eleven properties, therefore, allowing the calculation of all properties from a single analysis.

3 Molecular Descriptors

There are 42 molecular descriptors (i.e. groups) in the Joback & Reid method [1]. These molecular descriptors are listed below, along with a short description and the name of the "MedeA variable" that is associated with each descriptor. MedeA variables are useful when printing these quantities in user-defined tables, as part of a flowchart involving a QSPR stage.

[1] Kevin G Joback and Robert C Reid, "Estimation of Pure-Component Properties From Group-Contributions," *Chemical Engineering Communications* 57, no. 1 (February 5, 1987): 233-243.

Table1: Descriptors, *MedeA* variables and a summary of each descriptor.

Descriptor	<i>MedeA</i> variable	Description
NC0	qspr_NC0.calc	-C atoms with zero contribution, member of another group
NC1	qspr_NC1.calc	-CH ₃ groups, non-ring
NC2	qspr_NC2.calc	-CH ₂ groups, non-ring
NC3	qspr_NC3.calc	-CH groups, non-ring
NC4	qspr_NC4.calc	-C atoms, non-ring
NC5	qspr_NC5.calc	=CH ₂ groups, non-ring
NC6	qspr_NC6.calc	=CH groups, non-ring
NC7	qspr_NC7.calc	=C atoms, non-ring
NC8	qspr_NC8.calc	=C= atoms, non-ring
NC9	qspr_NC9.calc	#CH groups, non-ring
NC10	qspr_NC10.calc	#C atoms, non-ring
NC11	qspr_NC11.calc	-CH ₂ non-aromatic groups, ring
NC12	qspr_NC12.calc	-CH non-aromatic groups, ring
NC13	qspr_NC13.calc	-C non-aromatic atoms, ring
NC14	qspr_NC14.calc	=CH aromatic groups, ring
NC15	qspr_NC15.calc	=C aromatic atoms, ring
NF1	qspr_NF1.calc	F atoms
NCI1	qspr_NCI1.calc	Cl atoms
NBr1	qspr_NBr1.calc	Br atoms
NI1	qspr_NI1.calc	I atoms
NO1	qspr_NO1.calc	-O- groups in OH, in alcohols
NO2	qspr_NO2.calc	-O- groups in OH, in phenol
NO3	qspr_NO3.calc	-O- groups in ethers, non-ring
NO4	qspr_NO4.calc	-O- groups in ethers, ring
NO5	qspr_NO5.calc	=O groups, non-ring
NO6	qspr_NO6.calc	=O groups, ring
NO7	qspr_NO7.calc	=O groups in aldehydes
NO8	qspr_NO8.calc	-O- groups in carboxylic acid groups
NO9	qspr_NO9.calc	-O- groups in carboxylic ester groups
NO10	qspr_NO10.calc	=O groups in other than NO1-NO9 groups
NN1	qspr_NN1.calc	-NH ₂ groups, in primary amines
NN2	qspr_NN2.calc	-NH groups, in secondary amines, non-ring
NN3	qspr_NN3.calc	-NH groups, in secondary amines, ring
NN4	qspr_NN4.calc	-N atoms in tertiary amines, non-ring
NN5	qspr_NN5.calc	-N= atoms, nonring
NN6	qspr_NN6.calc	-N= atoms, ring
NN7	qspr_NN7.calc	=NH groups
NN8	qspr_NN8.calc	CN- groups, in cyanides
NN9	qspr_NN9.calc	-NO ₂ groups
NS1	qspr_NS1.calc	-SH groups, in thiols
NS2	qspr_NS2.calc	-S atoms, non-ring
NS3	qspr_NS3.calc	-S- atoms, ring
NH1	qspr_NH1.calc	-H atoms with zero contribution, member of another group

4 Properties

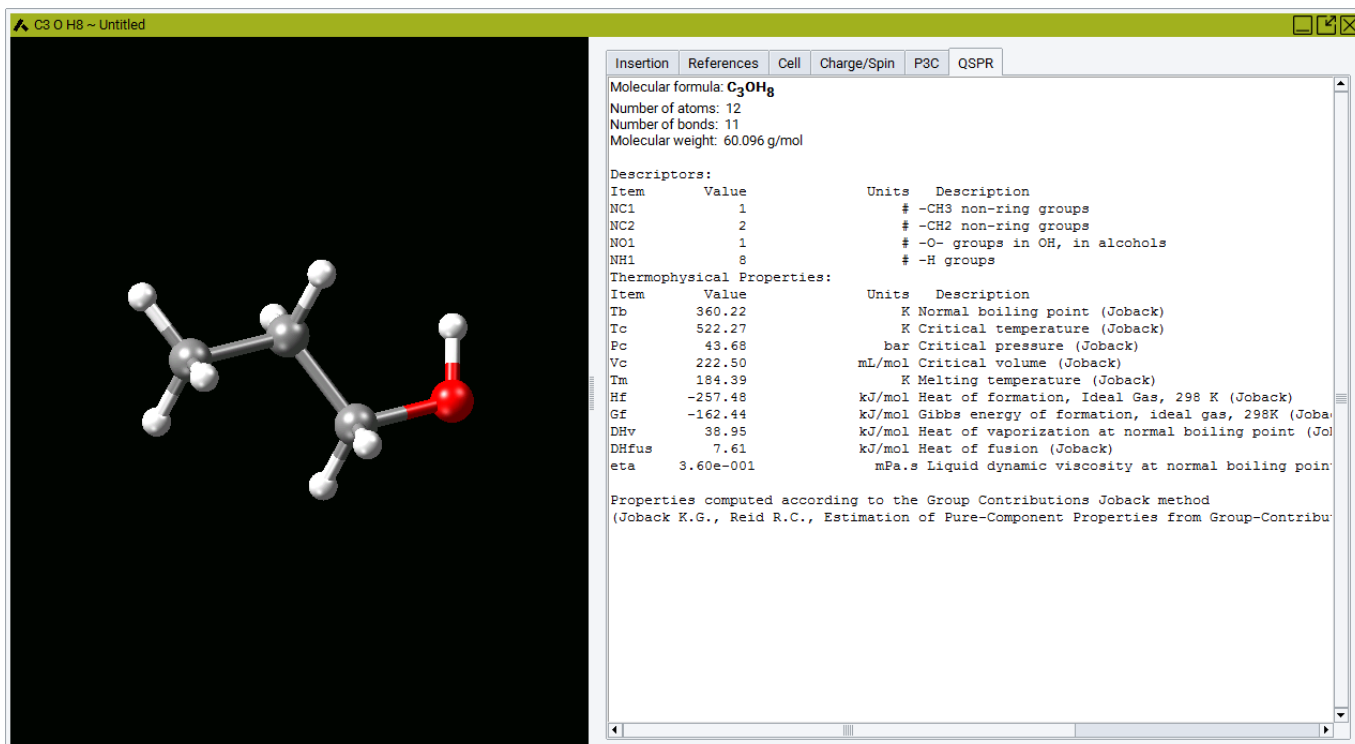
There are ten properties calculated using the Joback & Reid method [1].

Table2: Properties, *Medea* variables and a description of each property.

Property	Units	<i>Medea</i> variable	Description
Tb	K	qspr_Tb_calc	Normal Boiling Point Temperature
Tc	K	qspr_Tc_calc	Critical Temperature
Pc	bar	qspr_Pc_calc	Critical Pressure
Vc	ml/mol	qspr_Vc_calc	Critical Volume
Tm	K	qspr_Tm_calc	Melting Temperature
Hf	kJ/mol	qspr_Hf_calc	Heat of Formation, ideal gas, 298 K
Gf	kJ/mol	qspr_Gf_calc	Gibbs Energy of Formation, ideal gas, 298 K
DHv	kJ/mol	qspr_DHv_calc	Heat of Vaporization at normal boiling point
DHfus	kJ/mol	qspr_DHfus_calc.	Heat of Fusion
Eta	mPas	qspr_eta_calc	Liquid Dynamic Viscosity at normal boiling point

Both the molecular descriptors and the calculated properties are available interactively in the *Molecular Builder*, or through a **QSPR: Property Prediction using Group Contributions** stage in a *Medea* flowchart.

The results for propanol appear as shown here on the *QSPR* tab of the *Molecular Builder* and the output of a **QSPR: Property Prediction using Group Contributions** stage looks like this in *Job.out*.



C3 O H8 ~ Untitled

Insertion References Cell Charge/Spin P3C QSPR

Molecular formula: **C₃H₈O**
 Number of atoms: 12
 Number of bonds: 11
 Molecular weight: 60.096 g/mol

Descriptors:

Item	Value	Units	Description
NC1	1	#	-CH3 non-ring groups
NC2	2	#	-CH2 non-ring groups
NO1	1	#	-O- groups in OH, in alcohols
NH1	8	#	-H groups

Thermophysical Properties:

Item	Value	Units	Description
Tb	360.22	K	Normal boiling point (Joback)
Tc	522.27	K	Critical temperature (Joback)
Pc	43.68	bar	Critical pressure (Joback)
Vc	222.50	mL/mol	Critical volume (Joback)
Tm	184.39	K	Melting temperature (Joback)
Hf	-257.48	kJ/mol	Heat of formation, Ideal Gas, 298 K (Joback)
Gf	-162.44	kJ/mol	Gibbs energy of formation, ideal gas, 298K (Joback)
DHv	38.95	kJ/mol	Heat of vaporization at normal boiling point (Joback)
DHfus	7.61	kJ/mol	Heat of fusion (Joback)
eta	3.60e-001	mPa.s	Liquid dynamic viscosity at normal boiling point (Joback)

Properties computed according to the Group Contributions Joback method
 (Joback K.G., Reid R.C., Estimation of Pure-Component Properties from Group-Contribu

Stage 1: Property Prediction using Group Contributions

Molecular formula: C30H8
 Number of atoms: 12
 Number of bonds: 11
 Molecular weight: 60.096 g/mol

Descriptors:

Item	Value	Units	Description
NC1	1	#	-CH3 non-ring groups
NC2	2	#	-CH2 non-ring groups
NO1	1	#	-O- groups in OH, in alcohols
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(Joback K.G., Reid R.C., Estimation of Pure-Component Properties from Group-Contributions, Chem. Eng. Commun. 57, p. 233-243 (1987))

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