Dihydrosinapyl alcohol

Other names: 1-(4-Hydroxy-3,5-dimethoxyphenyl)-1-propanol (dihydrosinapyl alcohol)
1-Propanol, 3-(4-hydroxy-3,5-dimethoxyphenyl)
Inchi: InChI=1S/C11H16O4/c1-14-9-6-8(4-3-5-12)7-10(15-2)11(9)13/h6-7,12-13H,3-5H2,1-2H3
InchiKey: PHOPGVYKZWPIGA-UHFFFAOYSA-N
Formula: C11H16O4
SMILES: COc1cc(CCCO)cc(OC)c1O
Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
gf	-366.55	kJ/mol	Joback Method
hf	-650.76	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.334		Crippen Method
mcvol	165.570	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	705.36	K	Joback Method
tc	904.51	K	Joback Method
tf	482.19	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.30	J/mol×K	705.36	Joback Method
cpg	468.57	J/mol×K	738.55	Joback Method
cpg	479.30	J/mol×K	771.74	Joback Method
cpg	489.50	J/mol×K	804.93	Joback Method
cpg	499.20	J/mol×K	838.13	Joback Method
cpg	508.43	J/mol×K	871.32	Joback Method

cpg	517.22	J/mol×K	904.51	Joback Method
dvisc	0.0001440	Pa×s	482.19	Joback Method
dvisc	0.0000613	Pa×s	519.38	Joback Method
dvisc	0.0000292	Pa×s	556.58	Joback Method
dvisc	0.0000153	Pa×s	593.78	Joback Method
dvisc	0.0000086	Pa×s	630.97	Joback Method
dvisc	0.0000052	Pa×s	668.16	Joback Method
dvisc	0.0000033	Pa×s	705.36	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R88372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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