Guaifenesin M (OH)

Inchi: InChI=1S/C9H12O5/c10-4-7(12)5-14-9-2-1-6(11)3-8(9)13/h1-3,7,10-13H,4-5H2
InchiKey: KTVVVQFVVLMWAL-UHFFFAOYSA-N
Formula: C9H12O5
SMILES: OCC(O)COc1ccc(O)cc1O
Mol. weight [g/mol]: 200.19

Physical Properties

Property code	Value	Unit	Source
gf	-553.01	kJ/mol	Joback Method
hf	-789.14	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	-0.170		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
rinpol	2235.00		NIST Webbook
tb	799.58	K	Joback Method
tc	1005.81	K	Joback Method
tf	569.92	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.14	J/mol×K	799.58	Joback Method
cpg	429.09	J/mol×K	833.95	Joback Method
cpg	436.86	J/mol×K	868.32	Joback Method
cpg	444.51	J/mol×K	902.69	Joback Method
cpg	452.14	J/mol×K	937.07	Joback Method
cpg	459.84	J/mol×K	971.44	Joback Method
cpg	467.68	J/mol×K	1005.81	Joback Method
dvisc	0.0000042	Pa×s	569.92	Joback Method
dvisc	0.0000014	Pa×s	608.20	Joback Method

dvisc	0.0000005	Pa×s	646.47	Joback Method
dvisc	0.0000002	Pa×s	684.75	Joback Method
dvisc	0.0000001	Pa×s	723.03	Joback Method
dvisc	5.4879783e-08	Pa×s	761.30	Joback Method
dvisc	2.9604174e-08	Pa×s	799.58	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=R57470&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