Guaifenesin M (des-methyl)

Inchi: InChI=1S/C9H12O4/c10-5-7(11)6-13-9-4-2-1-3-8(9)12/h1-4,7,10-12H,5-6H2
InchiKey: YFTRBASNPFHPAJ-UHFFFAOYSA-N
Formula: C9H12O4
SMILES: OCC(O)COc1ccccc1O
Mol. weight [g/mol]: 184.19

Physical Properties

Property code	Value	Unit	Source
gf	-398.39	kJ/mol	Joback Method
hf	-611.83	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.124		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
rinpol	1920.00		NIST Webbook
tb	718.96	K	Joback Method
tc	915.69	K	Joback Method
tf	458.20	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.04	J/mol×K	718.96	Joback Method
cpg	390.61	J/mol×K	751.75	Joback Method
cpg	398.72	J/mol×K	784.54	Joback Method
cpg	406.42	J/mol×K	817.32	Joback Method
cpg	413.75	J/mol×K	850.11	Joback Method
cpg	420.77	J/mol×K	882.90	Joback Method
cpg	427.51	J/mol×K	915.69	Joback Method
dvisc	0.0003171	Pa×s	458.20	Joback Method
dvisc	0.0000797	Pa×s	501.66	Joback Method

dvisc	0.0000250	Pa×s	545.12	Joback Method
dvisc	0.0000093	Pa×s	588.58	Joback Method
dvisc	0.0000040	Pa×s	632.04	Joback Method
dvisc	0.0000019	Pa×s	675.50	Joback Method
dvisc	0.0000010	Pa×s	718.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R57466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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