1-hydroxy-(1-methoxy)-7-(methylethyl)[1,2,3,3«alp

Inchi: InChI=1S/C13H22O/c1-9(2)11-5-3-4-10-6-7-13(14)12(10)8-11/h8-11,13-14H,3-7H2,1-2H
InchiKey: ZKWSHMCGJMCXMN-UHFFFAOYSA-N
Formula: C13H22O
SMILES: CC(C)C1C=C2C(O)CCC2CCC1
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	5.04	kJ/mol	Joback Method
hf	-322.23	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	61.98	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.140		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	618.61	K	Joback Method
tc	822.69	K	Joback Method
tf	312.93	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.00	J/mol×K	618.61	Joback Method
cpg	575.31	J/mol×K	788.68	Joback Method
cpg	560.49	J/mol×K	754.66	Joback Method
cpg	544.70	J/mol×K	720.65	Joback Method
cpg	527.88	J/mol×K	686.64	Joback Method
cpg	509.99	J/mol×K	652.62	Joback Method
cpg	589.20	J/mol×K	822.69	Joback Method
dvisc	0.0001402	Pa×s	618.61	Joback Method

dvisc	0.0002081	Pa×s	567.66	Joback Method
dvisc	0.0003337	Pa×s	516.72	Joback Method
dvisc	0.0005933	Pa×s	465.77	Joback Method
dvisc	0.0012152	Pa×s	414.82	Joback Method
dvisc	0.0030423	Pa×s	363.88	Joback Method
dvisc	0.0102693	Pa×s	312.93	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=R519941&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