

Dihydrosesquicineole

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H28O/c1-12(2)6-5-9-15(4)13-7-10-14(3,16-15)11-8-13/h12-13H,5-11H2,1-4H

ANKKQGMQMYAVFB-FGRDXJNISA-N

C15H28O

CC(C)CCCC1(C)OC2(C)CCC1CC2

224.38

Physical Properties

Property code	Value	Unit	Source
gf	65.47	kJ/mol	Joback Method
hf	-346.79	kJ/mol	Joback Method
hfus	19.61	kJ/mol	Joback Method
hvap	50.67	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.550		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
ripol	1794.00		NIST Webbook
ripol	1794.00		NIST Webbook
tb	586.94	K	Joback Method
tc	796.45	K	Joback Method
tf	342.78	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.46	J/mol×K	586.94	Joback Method
cpg	593.60	J/mol×K	621.86	Joback Method
cpg	614.46	J/mol×K	656.78	Joback Method
cpg	634.25	J/mol×K	691.70	Joback Method
cpg	653.21	J/mol×K	726.61	Joback Method
cpg	671.55	J/mol×K	761.53	Joback Method
cpg	689.49	J/mol×K	796.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R517618&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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