Dehydro-sesquicineole

Other names: Dehydrosesquicineol
Inchi: InChI=1S/C15H24O/c1-12(2)6-5-9-15(4)13-7-10-14(3,16-15)11-8-13/h6-7,10,13H,5,8-9,1
InchiKey: VLUGOADEEDGFLB-GRKKQISMSA-N
Formula: C15H24O
SMILES: CC(C)=CCCC1(C)OC2(C)C=CC1CC2
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	169.54	kJ/mol	Joback Method
hf	-176.30	kJ/mol	Joback Method
hfus	23.24	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1461.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1823.00		NIST Webbook
tb	590.58	K	Joback Method
tc	810.51	K	Joback Method
tf	339.50	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.24	J/mol×K	590.58	Joback Method
cpg	551.82	J/mol×K	627.23	Joback Method
cpg	571.11	J/mol×K	663.89	Joback Method
cpg	589.38	J/mol×K	700.54	Joback Method
cpg	606.90	J/mol×K	737.20	Joback Method
cpg	623.95	J/mol×K	773.85	Joback Method

cpg	640.79	J/mol×K	810.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288172&Units=SI
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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume