Sesquicineole

Inchi: InChI=1S/C15H26O/c1-12(2)6-5-9-15(4)13-7-10-14(3,16-15)11-8-13/h6,13H,5,7-11H2,1-
InchiKey: BAQRIYKLDIPFQB-JNNQLUTISA-N
Formula: C15H26O
SMILES: CC(C)=CCCC1(C)OC2(C)CCC1CC2
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	139.58	kJ/mol	Joback Method
hf	-234.08	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.471		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1516.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1733.00		NIST Webbook
tb	591.42	K	Joback Method

tc	809.30	K	Joback Method
tf	338.74	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.75	J/mol×K	591.42	Joback Method
cpg	573.41	J/mol×K	627.73	Joback Method
cpg	593.76	J/mol×K	664.05	Joback Method
cpg	613.05	J/mol×K	700.36	Joback Method
cpg	631.55	J/mol×K	736.67	Joback Method
cpg	649.52	J/mol×K	772.99	Joback Method
cpg	667.22	J/mol×K	809.30	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R199270&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