Lanceol, cis

Other names: (Z)-Lanceol
cis-Lanceol
Inchi: InChI=1S/C15H24O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5,7,15-16H,3-4,6,8-11
InchiKey: HBVOEGGRCJCMLG-ACAGNQJTSA-N
Formula: C15H24O
SMILES: C=C(CCC=C(C)CO)C1CC=C(C)CC1
Mol. weight [g/mol]: 220.35
CAS: 10067-28-4

Physical Properties

Property code	Value	Unit	Source
gf	134.34	kJ/mol	Joback Method
hf	-181.46	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1763.90		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1766.10		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
ripol	2453.00		NIST Webbook
ripol	2518.00		NIST Webbook
ripol	2518.00		NIST Webbook
ripol	2518.00		NIST Webbook

tb	659.07	K	Joback Method
tc	853.50	K	Joback Method
tf	305.53	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.70	J/mol×K	659.07	Joback Method
cpg	580.78	J/mol×K	691.47	Joback Method
cpg	596.91	J/mol×K	723.88	Joback Method
cpg	612.15	J/mol×K	756.28	Joback Method
cpg	626.54	J/mol×K	788.69	Joback Method
cpg	640.14	J/mol×K	821.09	Joback Method
cpg	652.98	J/mol×K	853.50	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=C10067284&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

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