Lanceol oxide

Inchi: InChI=1S/C14H22O/c1-11-6-8-13(9-7-11)14-5-3-4-12(2)10-15-14/h4,6,13-14H,3,5,7-10H
InchiKey: QTWUDCCAKQVTQQ-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC1=CCC(C2CCC=C(C)CO2)CC1
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	58.34	kJ/mol	Joback Method
hf	-269.19	kJ/mol	Joback Method
hfus	23.23	kJ/mol	Joback Method
hvap	54.21	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.858		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	598.32	K	Joback Method
tc	833.87	K	Joback Method
tf	311.91	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.57	J/mol×K	598.32	Joback Method
cpg	514.22	J/mol×K	637.58	Joback Method
cpg	536.34	J/mol×K	676.84	Joback Method
cpg	556.95	J/mol×K	716.10	Joback Method
cpg	576.09	J/mol×K	755.36	Joback Method
cpg	593.79	J/mol×K	794.62	Joback Method
cpg	610.10	J/mol×K	833.87	Joback Method
dvisc	0.0035446	Pa×s	311.91	Joback Method

dvisc	0.0014984	Pa×s	359.64	Joback Method
dvisc	0.0007750	Pa×s	407.38	Joback Method
dvisc	0.0004603	Pa×s	455.11	Joback Method
dvisc	0.0003018	Pa×s	502.85	Joback Method
dvisc	0.0002129	Pa×s	550.58	Joback Method
dvisc	0.0001588	Pa×s	598.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407239&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
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