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«alpha»,13-Epoxy-14,15,16-trinorlabdan-13-one

Inchi:	InChI=1S/C16H26O2/c1-15(2)9-4-10-16(3)11-5-8-14(17)18-12(11)6-7-13(15)16/h11-13H
InchiKey:	TVZBUIHFVNFNKU-UWTNAYQSSA-N
Formula:	C16H26O2
SMILES:	CC1(C)CCCC2(C)C3CCC(=O)OC3CCC12
Mol. weight [g/mol]:	250.38

Physical Properties

Property code	Value	Unit	Source
gf	-29.52	kJ/mol	Joback Method
hf	-465.87	kJ/mol	Joback Method
hfus	18.14	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.935		Crippen Method
mcvol	211.160	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
ripol	2764.00		NIST Webbook
tb	692.96	K	Joback Method
tc	943.53	K	Joback Method
tf	440.41	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.47	J/mol×K	692.96	Joback Method
cpg	690.07	J/mol×K	734.72	Joback Method
cpg	714.52	J/mol×K	776.48	Joback Method
cpg	738.16	J/mol×K	818.24	Joback Method
cpg	761.30	J/mol×K	860.00	Joback Method
cpg	784.28	J/mol×K	901.76	Joback Method
cpg	807.41	J/mol×K	943.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R344153&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
mccvol:	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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