8,13-Epoxy-15,16-dinorlabd-12-ene

Inchi: InChI=1S/C17H28O/c1-12-6-7-13-14(18-12)8-9-15-16(2,3)10-5-11-17(13,15)4/h6,13-15H
InchiKey: WZENFBKOQYBKCE-FKFDDHQTSA-N
Formula: C17H28O
SMILES: CC1=CCC2C(CCC3C(C)(C)CCCC23C)O1
Mol. weight [g/mol]: 248.40

Physical Properties

Property code	Value	Unit	Source
gf	121.82	kJ/mol	Joback Method
hf	-302.50	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.922		Crippen Method
mcvol	219.380	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		NIST Webbook
tb	652.16	K	Joback Method
tc	889.23	K	Joback Method
tf	396.74	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.09	J/mol×K	652.16	Joback Method
cpg	680.52	J/mol×K	691.67	Joback Method
cpg	704.61	J/mol×K	731.18	Joback Method
cpg	727.69	J/mol×K	770.69	Joback Method
cpg	750.06	J/mol×K	810.20	Joback Method

cpg	772.04	J/mol×K	849.72	Joback Method
cpg	793.95	J/mol×K	889.23	Joback Method

Sources

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=R336053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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