1,10-Epoxigermacrene D

Inchi: InChI=1S/C15H24O/c1-11(2)13-7-5-12(3)6-8-14-15(4,16-14)10-9-13/h5,7,11,13-14H,3,6,
InchiKey: YWGIUJSFKKGYFZ-PFGKWIECSA-N
Formula: C15H24O
SMILES: C=C1C=CC(C(C)C)CCC2(C)OC2CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	117.70	kJ/mol	Joback Method
hf	-238.49	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.103		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	597.83	K	Joback Method
tc	824.87	K	Joback Method
tf	322.76	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.26	J/mol×K	597.83	Joback Method
cpg	560.48	J/mol×K	635.67	Joback Method
cpg	582.27	J/mol×K	673.51	Joback Method
cpg	602.77	J/mol×K	711.35	Joback Method
cpg	622.13	J/mol×K	749.19	Joback Method
cpg	640.50	J/mol×K	787.03	Joback Method
cpg	658.03	J/mol×K	824.87	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=R408603&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume