cis-4,10-epoxy-Amorphane

Inchi: InChI=1S/C15H26O/c1-10(2)11-5-8-15(4)13-6-7-14(3,16-15)9-12(11)13/h10-13H,5-9H2,1
InchiKey: GRFWMFZRMJAPKB-HTXSYXIBSA-N
Formula: C15H26O
SMILES: CC(C)C1CCC2(C)OC3(C)CCC2C1C3
Mol. weight [g/mol]: 222.37
CAS: 70470-08-5

Physical Properties

Property code	Value	Unit	Source
gf	118.51	kJ/mol	Joback Method
hf	-294.33	kJ/mol	Joback Method
hfus	18.81	kJ/mol	Joback Method
hvap	50.27	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1482.00		NIST Webbook
tb	589.01	K	Joback Method
tc	813.73	K	Joback Method
tf	356.48	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.13	J/mol×K	589.01	Joback Method
cpg	582.85	J/mol×K	626.46	Joback Method
cpg	605.04	J/mol×K	663.92	Joback Method
cpg	625.99	J/mol×K	701.37	Joback Method
cpg	646.00	J/mol×K	738.82	Joback Method
cpg	665.37	J/mol×K	776.27	Joback Method
cpg	684.40	J/mol×K	813.73	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=C70470085&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