(+)-(1R,2S,6R,8S,10S)-2,8-Epoxyamorpha-4,7(11)-d

Inchi: InChI=1S/C15H22O/c1-8(2)14-11-5-9(3)6-12-15(11)10(4)7-13(14)16-12/h5,10-13,15H,6-
InchiKey: HWBVMESCZGIWFV-KMCWBVRRSA-N
Formula: C15H22O
SMILES: CC1=CC2C(=C(C)C)C3CC(C)C2C(C1)O3
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	189.17	kJ/mol	Joback Method
hf	-206.98	kJ/mol	Joback Method
hfus	34.78	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.712		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	599.63	K	Joback Method
tc	816.32	K	Joback Method
tf	333.36	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.85	J/mol×K	599.63	Joback Method
cpg	544.19	J/mol×K	635.75	Joback Method
cpg	564.19	J/mol×K	671.86	Joback Method
cpg	582.95	J/mol×K	707.98	Joback Method
cpg	600.56	J/mol×K	744.09	Joback Method
cpg	617.10	J/mol×K	780.21	Joback Method
cpg	632.68	J/mol×K	816.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515776&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
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