

6,11-Epoxyguaia-4,9-diene

Inchi:	InChI=1S/C15H22O/c1-9-5-6-12-10(2)7-11-8-13(14(9)12)16-15(11,3)4/h7,11-13H,5-6,8H
InchiKey:	SVGQUABWMVWDON-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC1=CC2CC(OC2(C)C)C2=C(C)CCC12
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	153.08	kJ/mol	Joback Method
hf	-208.96	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mvol	186.900	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	611.41	K	Joback Method
tc	837.39	K	Joback Method
tf	387.38	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.31	J/mol×K	611.41	Joback Method
cpg	542.04	J/mol×K	649.07	Joback Method
cpg	561.52	J/mol×K	686.74	Joback Method
cpg	579.93	J/mol×K	724.40	Joback Method
cpg	597.46	J/mol×K	762.07	Joback Method
cpg	614.29	J/mol×K	799.73	Joback Method
cpg	630.61	J/mol×K	837.39	Joback Method

Sources

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=R232763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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