

exo-1,5-Epoxyalvial-4(14)-ene

Inchi:	InChI=1S/C15H24O/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(16-12)13(11)15/h9,11-14H,3,5-8
InchiKey:	BITBXAWCPCNKKN-JSPOSNOBSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2OC1C1C(C(C)C)CCC21C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	177.08	kJ/mol	Joback Method
hf	-225.33	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.792		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1548.00		NIST Webbook
ripol	1945.00		NIST Webbook
tb	587.93	K	Joback Method
tc	805.89	K	Joback Method
tf	346.26	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.56	J/molxK	587.93	Joback Method
cpg	562.18	J/molxK	624.26	Joback Method
cpg	583.38	J/molxK	660.58	Joback Method
cpg	603.34	J/molxK	696.91	Joback Method
cpg	622.22	J/molxK	733.23	Joback Method
cpg	640.21	J/molxK	769.56	Joback Method
cpg	657.47	J/molxK	805.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R201259&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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