

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-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2OC1C1C(C(C)C)CCC21C
Mol. weight [g/mol]:	220.35
CAS:	88395-47-5

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	1571.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1573.50		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1573.50		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1576.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1950.00		NIST Webbook

ripol	1945.00		NIST Webbook
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ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1924.00		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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.56	J/mol×K	587.93	Joback Method
cpg	562.18	J/mol×K	624.26	Joback Method
cpg	583.38	J/mol×K	660.58	Joback Method
cpg	603.34	J/mol×K	696.91	Joback Method
cpg	622.22	J/mol×K	733.23	Joback Method
cpg	640.21	J/mol×K	769.56	Joback Method
cpg	657.47	J/mol×K	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=C88395475&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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