Farnesene epoxide, E-

Other names: (E)-«beta»-Farnesene epoxide: (E)-(5,9)-Dimethyl-1-methylene-4,8-decadienyl)oxirane
Inchi: InChI=1S/C15H24O/c1-12(2)7-5-8-13(3)9-6-10-14(4)15-11-16-15/h7,9,15H,4-6,8,10-11H
InchiKey: HNYSBTOKKSTMIG-UKTHLTGXSA-N
Formula: C15H24O
SMILES: C=C(CCC=C(C)CCC=C(C)C)C1CO1
Mol. weight [g/mol]: 220.35
CAS: 83637-40-5

Physical Properties

Property code	Value	Unit	Source
gf	272.68	kJ/mol	Joback Method
hf	-81.63	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	52.89	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.414		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	580.93	K	Joback Method
tc	775.61	K	Joback Method
tf	249.52	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.36	J/mol×K	580.93	Joback Method
cpg	541.86	J/mol×K	613.38	Joback Method
cpg	559.29	J/mol×K	645.82	Joback Method
cpg	575.73	J/mol×K	678.27	Joback Method
cpg	591.27	J/mol×K	710.72	Joback Method
cpg	605.97	J/mol×K	743.16	Joback Method
cpg	619.92	J/mol×K	775.61	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=C83637405&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