Epoxybulnesene

Inchi: InChI=1S/C15H24O/c1-10(2)12-6-7-14(4)15(16-14)8-5-11(3)13(15)9-12/h11-13H,1,5-9H
InchiKey: OQZCYVPJJHEMSP-PBWBXLIUSA-N
Formula: C15H24O
SMILES: C=C(C)C1CCC2(C)OC23CCC(C)C3C1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	200.24	kJ/mol	Joback Method
hf	-173.41	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	586.01	K	Joback Method
tc	814.79	K	Joback Method
tf	355.76	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.32	J/mol×K	586.01	Joback Method
cpg	560.41	J/mol×K	624.14	Joback Method
cpg	581.93	J/mol×K	662.27	Joback Method
cpg	602.21	J/mol×K	700.40	Joback Method
cpg	621.57	J/mol×K	738.53	Joback Method
cpg	640.32	J/mol×K	776.66	Joback Method

cpg	658.78	J/mol×K	814.79	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=R612996&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
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