trans-2-«alpha»-bisabolene epoxide

Inchi: InChI=1S/C15H24O/c1-11(2)5-10-14-15(4,16-14)13-8-6-12(3)7-9-13/h5-6,13-14H,7-10H2
InchiKey: PBNXUEQZNAEDOI-NOYMGPGASA-N
Formula: C15H24O
SMILES: CC(C)=CCC1OC1(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	153.30	kJ/mol	Joback Method
hf	-209.17	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.247		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
ripol	1999.00		NIST Webbook
tb	599.59	K	Joback Method
tc	819.43	K	Joback Method
tf	324.60	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.36	J/mol×K	599.59	Joback Method
cpg	556.81	J/mol×K	636.23	Joback Method
cpg	576.95	J/mol×K	672.87	Joback Method
cpg	595.97	J/mol×K	709.51	Joback Method
cpg	614.03	J/mol×K	746.15	Joback Method
cpg	631.29	J/mol×K	782.79	Joback Method
cpg	647.92	J/mol×K	819.43	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=R402823&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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