E-Piperetone epoxide

Inchi: InChI=1S/C11H18O/c1-7(2)9-5-6-11(4)10(12-11)8(9)3/h7,9-10H,3,5-6H2,1-2,4H3/t9-,10-
InchiKey: VKGXTTWOABBGQO-MXWKQRLJSA-N
Formula: C11H18O
SMILES: C=C1C(C(C)C)CCC2(C)OC12
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	102.46	kJ/mol	Joback Method
hf	-189.07	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	42.90	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.766		Crippen Method
mcvol	145.700	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	490.07	K	Joback Method
tc	698.76	K	Joback Method
tf	291.00	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.99	J/mol×K	490.07	Joback Method
cpg	369.46	J/mol×K	524.85	Joback Method
cpg	386.66	J/mol×K	559.63	Joback Method
cpg	402.72	J/mol×K	594.42	Joback Method
cpg	417.78	J/mol×K	629.20	Joback Method
cpg	431.96	J/mol×K	663.98	Joback Method
cpg	445.40	J/mol×K	698.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420905&Units=SI
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

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