Peculiaroxide

Inchi: InChI=1S/C15H26O/c1-10-8-13(2,3)12-9-14(4)7-6-11(12)15(10,5)16-14/h10-12H,6-9H2,1
InchiKey: IQWAWENFFQLNLN-LZVAUXPFSA-N
Formula: C15H26O
SMILES: CC1CC(C)(C)C2CC3(C)CCC2C1(C)O3
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	107.75	kJ/mol	Joback Method
hf	-294.15	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	49.20	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1413.00		NIST Webbook
tb	585.02	K	Joback Method
tc	813.84	K	Joback Method
tf	391.14	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.85	J/mol×K	585.02	Joback Method
cpg	581.52	J/mol×K	623.16	Joback Method
cpg	603.66	J/mol×K	661.29	Joback Method
cpg	624.68	J/mol×K	699.43	Joback Method
cpg	644.99	J/mol×K	737.57	Joback Method
cpg	664.97	J/mol×K	775.71	Joback Method
cpg	685.05	J/mol×K	813.84	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=R413348&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