4-(1-Hydroperoxy-2,2-dimethyl-6-methylene-cyclo

Inchi: InChI=1S/C14H22O3/c1-10-7-6-8-13(4,5)14(10,17-16)11(2)9-12(3)15/h9,16H,1,6-8H2,2-
InchiKey: ABKYIBLLJAHNQO-PKNBQFBNSA-N
Formula: C14H22O3
SMILES: C=C1CCCC(C)(C)C1(OO)C(C)=CC(C)=O
Mol. weight [g/mol]: 238.32
CAS: 125284-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-173.23	kJ/mol	Joback Method
hf	-473.19	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.516		Crippen Method
mcvol	201.970	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
tb	706.75	K	Joback Method
tc	913.95	K	Joback Method
tf	426.10	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.64	J/mol×K	706.75	Joback Method
cpg	592.62	J/mol×K	741.28	Joback Method
cpg	608.20	J/mol×K	775.82	Joback Method
cpg	623.55	J/mol×K	810.35	Joback Method
cpg	638.84	J/mol×K	844.88	Joback Method
cpg	654.24	J/mol×K	879.42	Joback Method
cpg	669.94	J/mol×K	913.95	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=C125284200&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