Hydroperoxide, hexyl

Other names:	Hexyl hydroperoxide
	n-C6H13OOH
	1-Hydroperoxyhexane
Inchi:	InChI=1S/C6H14O2/c1-2-3-4-5-6-8-7/h7H,2-6H2,1H3
InchiKey:	RZICEOJUAFHYFO-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCCCCCOO
Mol. weight [g/mol]:	118.17
CAS:	4312-76-9

Physical Properties

Property code	Value	Unit	Source
chl	-4062.00 ± 5.00	kJ/mol	NIST Webbook
gf	-344.27	kJ/mol	Joback Method
hf	-517.44	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	46.11	kJ/mol	Joback Method
ie	9.47 ± 0.03	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
log10ws	-1.74		Crippen Method
logp	2.056		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	482.19	K	Joback Method
tc	671.20	K	Joback Method
tf	317.98	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.87	J/mol×K	482.19	Joback Method
cpg	271.15	J/mol×K	639.70	Joback Method
cpg	262.98	J/mol×K	608.20	Joback Method

cpg	254.38	J/mol×K	576.70	Joback Method
cpg	245.34	J/mol×K	545.19	Joback Method
cpg	235.84	J/mol×K	513.69	Joback Method
cpg	278.92	J/mol×K	671.20	Joback Method
dvisc	0.0002997	Pa×s	482.19	Joback Method
dvisc	0.0003680	Pa×s	454.82	Joback Method
dvisc	0.0004638	Pa×s	427.45	Joback Method
dvisc	0.0006034	Pa×s	400.09	Joback Method
dvisc	0.0008160	Pa×s	372.72	Joback Method
dvisc	0.0011576	Pa×s	345.35	Joback Method
dvisc	0.0017439	Pa×s	317.98	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=C4312769&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume