Hydroperoxide, 1-methylpentyl

Other names:	2-Hexyl hydroperoxide
	1-Methylpentyl hydroperoxide
	n-C4H9CH(CH3)OOH
	2-Hydroperoxyhexane
Inchi:	InChI=1S/C6H14O2/c1-3-4-5-6(2)8-7/h6-7H,3-5H2,1-2H3
InchiKey:	XWXUHAUZCICPHE-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CCCCC(C)OO
Mol. weight [g/mol]:	118.17
CAS:	24254-55-5

Physical Properties

Property code	Value	Unit	Source
chl	-4052.00 ± 3.00	kJ/mol	NIST Webbook
gf	-244.62	kJ/mol	Joback Method
hf	-456.90	kJ/mol	Joback Method
hfus	13.05	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
ie	9.96	eV	NIST Webbook
ie	9.25 ± 0.03	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	2.055		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	450.84	K	Joback Method
tc	615.45	K	Joback Method
tf	225.43	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.32	J/mol×K	450.84	Joback Method
cpg	275.39	J/mol×K	588.02	Joback Method

cpg	266.99	J/mol×K	560.58	Joback Method
cpg	258.28	J/mol×K	533.15	Joback Method
cpg	249.26	J/mol×K	505.71	Joback Method
cpg	239.95	J/mol×K	478.28	Joback Method
cpg	283.50	J/mol×K	615.45	Joback Method
dvisc	0.0001822	Pa×s	450.84	Joback Method
dvisc	0.0003176	Pa×s	413.27	Joback Method
dvisc	0.0006185	Pa×s	375.70	Joback Method
dvisc	0.0013969	Pa×s	338.13	Joback Method
dvisc	0.0038675	Pa×s	300.57	Joback Method
dvisc	0.0143235	Pa×s	263.00	Joback Method
dvisc	0.0820702	Pa×s	225.43	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24254555&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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