Hydroperoxide, 1-methylhexyl

Other names: n-C5H11CH(CH3)OOH
Inchi: InChI=1S/C7H16O2/c1-3-4-5-6-7(2)9-8/h7-8H,3-6H2,1-2H3
InchiKey: FWELUXZVATZEMI-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCCCCC(C)OO
Mol. weight [g/mol]: 132.20
CAS: 762-46-9

Physical Properties

Property code	Value	Unit	Source
chl	-4695.00 ± 2.00	kJ/mol	NIST Webbook
gf	-236.20	kJ/mol	Joback Method
hf	-477.54	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
ie	9.30 ± 0.03	eV	NIST Webbook
ie	9.94	eV	NIST Webbook
log10ws	-2.27		Crippen Method
logp	2.445		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	473.72	K	Joback Method
tc	637.45	K	Joback Method
tf	236.70	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.52	J/mol×K	473.72	Joback Method
cpg	321.47	J/mol×K	610.16	Joback Method
cpg	312.18	J/mol×K	582.87	Joback Method
cpg	302.54	J/mol×K	555.59	Joback Method
cpg	292.56	J/mol×K	528.30	Joback Method

cpg	282.22	J/mol×K	501.01	Joback Method
cpg	330.41	J/mol×K	637.45	Joback Method
dvisc	0.0001517	Pa×s	473.72	Joback Method
dvisc	0.0002622	Pa×s	434.22	Joback Method
dvisc	0.0005057	Pa×s	394.71	Joback Method
dvisc	0.0011285	Pa×s	355.21	Joback Method
dvisc	0.0030786	Pa×s	315.71	Joback Method
dvisc	0.0111917	Pa×s	276.20	Joback Method
dvisc	0.0625947	Pa×s	236.70	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=C762469&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

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