Hydroperoxide, 1-methylbutyl

Other names:	2-Hydroperoxypentane
	n-C3H7CH(CH3)OOH
Inchi:	InChI=1S/C5H12O2/c1-3-4-5(2)7-6/h5-6H,3-4H2,1-2H3
InchiKey:	XRIRVAYMWUMXBR-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CCCC(C)OO
Mol. weight [g/mol]:	104.15
CAS:	14018-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-253.04	kJ/mol	Joback Method
hf	-436.26	kJ/mol	Joback Method
hfus	10.46	kJ/mol	Joback Method
hvap	45.42	kJ/mol	Joback Method
ie	10.05	eV	NIST Webbook
ie	9.35 ± 0.03	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	1.665		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	855.00		NIST Webbook
rinpol	855.00		NIST Webbook
tb	427.96	K	Joback Method
tc	593.40	K	Joback Method
tf	214.16	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.34	J/mol×K	427.96	Joback Method
cpg	199.79	J/mol×K	455.53	Joback Method
cpg	207.98	J/mol×K	483.11	Joback Method

cpg	215.92	J/mol×K	510.68	Joback Method
cpg	223.60	J/mol×K	538.25	Joback Method
cpg	231.03	J/mol×K	565.83	Joback Method
cpg	238.21	J/mol×K	593.40	Joback Method
dvisc	0.1081645	Pa×s	214.16	Joback Method
dvisc	0.0183815	Pa×s	249.79	Joback Method
dvisc	0.0048625	Pa×s	285.43	Joback Method
dvisc	0.0017280	Pa×s	321.06	Joback Method
dvisc	0.0007551	Pa×s	356.69	Joback Method
dvisc	0.0003835	Pa×s	392.33	Joback Method
dvisc	0.0002180	Pa×s	427.96	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=C14018587&Units=SI

Legend

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume