

2-Hydroperoxy-n-hexane

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:	42081-81-2

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
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/molxK	450.84	Joback Method
cpg	239.95	J/molxK	478.28	Joback Method
cpg	249.26	J/molxK	505.71	Joback Method
cpg	258.28	J/molxK	533.15	Joback Method
cpg	266.99	J/molxK	560.58	Joback Method
cpg	275.39	J/molxK	588.02	Joback Method
cpg	283.50	J/molxK	615.45	Joback Method
dvisc	0.0820702	Paxs	225.43	Joback Method

dvisc	0.0143235	Paxs	263.00	Joback Method
dvisc	0.0038675	Paxs	300.57	Joback Method
dvisc	0.0013969	Paxs	338.13	Joback Method
dvisc	0.0006185	Paxs	375.70	Joback Method
dvisc	0.0003176	Paxs	413.27	Joback Method
dvisc	0.0001822	Paxs	450.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42081812&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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