

3-Hydroperoxy-n-heptane

Inchi:	InChI=1S/C7H16O2/c1-3-5-6-7(4-2)9-8/h7-8H,3-6H2,1-2H3
InchiKey:	RCPMMXGHMBPBLI-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCCC(CC)OO
Mol. weight [g/mol]:	132.20
CAS:	761-70-6

Physical Properties

Property code	Value	Unit	Source
chl	-4694.40 ± 4.20	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
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.52	J/mol×K	473.72	Joback Method
cpg	282.22	J/mol×K	501.01	Joback Method
cpg	292.56	J/mol×K	528.30	Joback Method
cpg	302.54	J/mol×K	555.59	Joback Method
cpg	312.18	J/mol×K	582.87	Joback Method
cpg	321.47	J/mol×K	610.16	Joback Method
cpg	330.41	J/mol×K	637.45	Joback Method
dvisc	0.0625947	Paxs	236.70	Joback Method

dvisc	0.0111917	Paxs	276.20	Joback Method
dvisc	0.0030786	Paxs	315.71	Joback Method
dvisc	0.0011285	Paxs	355.21	Joback Method
dvisc	0.0005057	Paxs	394.71	Joback Method
dvisc	0.0002622	Paxs	434.22	Joback Method
dvisc	0.0001517	Paxs	473.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C761706&Units=SI

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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