

Hydroperoxide, pentyl

Other names:	Pentyl hydroperoxide n-Amyl hydroperoxide Amyl hydroperoxide n-C5H11OOH
Inchi:	InChI=1S/C5H12O2/c1-2-3-4-5-7-6/h6H,2-5H2,1H3
InchiKey:	KCHNMIKAMRQBHD-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CCCCCOO
Mol. weight [g/mol]:	104.15
CAS:	74-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-352.69	kJ/mol	Joback Method
hf	-496.80	kJ/mol	Joback Method
hfus	18.85	kJ/mol	Joback Method
hvap	43.89	kJ/mol	Joback Method
ie	9.50 ± 0.30	eV	NIST Webbook
ie	9.83	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.666		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	459.31	K	Joback Method
tc	650.41	K	Joback Method
tf	306.71	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.92	J/mol×K	459.31	Joback Method
cpg	194.72	J/mol×K	491.16	Joback Method
cpg	203.10	J/mol×K	523.01	Joback Method

cpg	211.08	J/mol×K	554.86	Joback Method
cpg	218.66	J/mol×K	586.71	Joback Method
cpg	225.86	J/mol×K	618.56	Joback Method
cpg	232.70	J/mol×K	650.41	Joback Method
dvisc	0.0016683	Pa×s	306.71	Joback Method
dvisc	0.0011329	Pa×s	332.14	Joback Method
dvisc	0.0008129	Pa×s	357.58	Joback Method
dvisc	0.0006095	Pa×s	383.01	Joback Method
dvisc	0.0004737	Pa×s	408.44	Joback Method
dvisc	0.0003792	Pa×s	433.88	Joback Method
dvisc	0.0003112	Pa×s	459.31	Joback Method

Sources

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=C74806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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