

Hydroperoxide, 1-methylethyl

Other names:	Isopropyl hydroperoxide (CH ₃) ₂ CHOOH
Inchi:	InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3
InchiKey:	SGJUFIMCHSLMRJ-UHFFFAOYSA-N
Formula:	C ₃ H ₈ O ₂
SMILES:	CC(C)OO
Mol. weight [g/mol]:	76.09
CAS:	3031-75-2

Physical Properties

Property code	Value	Unit	Source
gf	-269.88	kJ/mol	Joback Method
hf	-197.10	kJ/mol	NIST Webbook
hfus	5.28	kJ/mol	Joback Method
hvap	40.97	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.884		Crippen Method
mvol	64.870	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	382.20	K	Joback Method
tc	548.82	K	Joback Method
tf	191.62	K	Joback Method
vc	0.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.53	J/molxK	382.20	Joback Method
cpg	126.27	J/molxK	409.97	Joback Method
cpg	131.87	J/molxK	437.74	Joback Method
cpg	137.33	J/molxK	465.51	Joback Method
cpg	142.65	J/molxK	493.28	Joback Method
cpg	147.83	J/molxK	521.05	Joback Method
cpg	152.86	J/molxK	548.82	Joback Method

dvisc	0.1898932	Paxs	191.62	Joback Method
dvisc	0.0303197	Paxs	223.38	Joback Method
dvisc	0.0076441	Paxs	255.15	Joback Method
dvisc	0.0026147	Paxs	286.91	Joback Method
dvisc	0.0011076	Paxs	318.67	Joback Method
dvisc	0.0005483	Paxs	350.44	Joback Method
dvisc	0.0003050	Paxs	382.20	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=C3031752&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
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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