

1-octen-3-hydroperoxide

Inchi:	InChI=1S/C8H16O2/c1-3-5-6-7-8(4-2)10-9/h4,8-9H,2-3,5-7H2,1H3
InchiKey:	CHGORMNWCVRPCH-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	C=CC(CCCCC)OO
Mol. weight [g/mol]:	144.21
CAS:	72755-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-139.94	kJ/mol	Joback Method
hf	-372.75	kJ/mol	Joback Method
hfus	16.95	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.611		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1127.00		NIST Webbook
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tb	493.28	K	Joback Method
tc	659.00	K	Joback Method
tf	246.21	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.02	J/molxK	493.28	Joback Method
cpg	348.45	J/molxK	631.38	Joback Method
cpg	338.96	J/molxK	603.76	Joback Method
cpg	329.08	J/molxK	576.14	Joback Method
cpg	318.80	J/molxK	548.52	Joback Method
cpg	308.11	J/molxK	520.90	Joback Method
cpg	357.56	J/molxK	659.00	Joback Method

dvisc	0.0001300	Paxs	493.28	Joback Method
dvisc	0.0002211	Paxs	452.10	Joback Method
dvisc	0.0004185	Paxs	410.92	Joback Method
dvisc	0.0009130	Paxs	369.75	Joback Method
dvisc	0.0024218	Paxs	328.57	Joback Method
dvisc	0.0084959	Paxs	287.39	Joback Method
dvisc	0.0453543	Paxs	246.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72755761&Units=SI
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

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

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