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
rinpol	1127.00		NIST Webbook
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/mol×K	493.28	Joback Method
cpg	348.45	J/mol×K	631.38	Joback Method
cpg	338.96	J/mol×K	603.76	Joback Method
cpg	329.08	J/mol×K	576.14	Joback Method
cpg	318.80	J/mol×K	548.52	Joback Method
cpg	308.11	J/mol×K	520.90	Joback Method
cpg	357.56	J/mol×K	659.00	Joback Method

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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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