2,5-Dimethylhexane-2,5-dihydroperoxide

Other names: Hydroperoxide, (1,1,4,4-tetramethyl-1,4-butanediyl)bis-
Inchi: InChI=1S/C8H18O4/c1-7(2,11-9)5-6-8(3,4)12-10/h9-10H,5-6H2,1-4H3
InchiKey: JGBAASVQPMTVHO-UHFFFAOYSA-N
Formula: C8H18O4
SMILES: CC(C)(CCC(C)(C)OO)OO
Mol. weight [g/mol]: 178.23
CAS: 3025-88-5

Physical Properties

Property code	Value	Unit	Source
gf	-461.48	kJ/mol	Joback Method
hf	-794.85	kJ/mol	Joback Method
hfs	-567.20 ± 3.50	kJ/mol	NIST Webbook
hfus	12.20	kJ/mol	Joback Method
hsub	138.60 ± 1.20	kJ/mol	NIST Webbook
hvap	68.99	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.303		Crippen Method
mcvol	147.060	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	605.18	K	Joback Method
tc	776.35	K	Joback Method
tf	350.86	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.53	J/mol×K	605.18	Joback Method
cpg	411.37	J/mol×K	633.71	Joback Method
cpg	421.67	J/mol×K	662.24	Joback Method
cpg	431.45	J/mol×K	690.77	Joback Method
cpg	440.73	J/mol×K	719.29	Joback Method
cpg	449.53	J/mol×K	747.82	Joback Method

cpg	457.87	J/mol×K	776.35	Joback Method
dvisc	0.0094291	Pa×s	350.86	Joback Method
dvisc	0.0018921	Pa×s	393.25	Joback Method
dvisc	0.0005190	Pa×s	435.63	Joback Method
dvisc	0.0001791	Pa×s	478.02	Joback Method
dvisc	0.0000735	Pa×s	520.41	Joback Method
dvisc	0.0000345	Pa×s	562.79	Joback Method
dvisc	0.0000180	Pa×s	605.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3025885&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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