2,5-Dihydroperoxy-2,5-dimethylhex-3-yne

Other names: Hydroperoxide, 1,1'-(1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis-

Hydroperoxide, (1,1,4,4-tetramethyl-2-butyne-1,4-diyl)bis-

Inchi: InChI=1S/C8H14O4/c1-7(2,11-9)5-6-8(3,4)12-10/h9-10H,1-4H3

InchiKey: VHRZZWMONXYKJP-UHFFFAOYSA-N

Formula: C8H14O4

SMILES: CC(C)(C#CC(C)(C)OO)OO

Mol. weight [g/mol]: 174.19

CAS: 3491-36-9

Physical Properties

Property code	Value	Unit	Source
chs	-4856.80	kJ/mol	NIST Webbook
gf	-258.68	kJ/mol	Joback Method
hf	-522.55	kJ/mol	Joback Method
hfs	-257.60 ± 2.80	kJ/mol	NIST Webbook
hfus	15.32	kJ/mol	Joback Method
hsub	127.40 ± 1.80	kJ/mol	NIST Webbook
hvap	71.14	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.526		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	614.18	K	Joback Method
tc	802.51	K	Joback Method
tf	456.96	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.45	J/mol×K	614.18	Joback Method
cpg	369.31	J/mol×K	645.57	Joback Method
cpg	378.64	J/mol×K	676.96	Joback Method
cpg	387.44	J/mol×K	708.35	Joback Method

cpg	395.74	J/mol×K	739.73	Joback Method
cpg	403.57	J/mol×K	771.12	Joback Method
cpg	410.94	J/mol×K	802.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3491369&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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

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