Dimethylvinylethynylhydroperoxide

Inchi: InChI=1S/C7H10O2/c1-4-5-6-7(2,3)9-8/h4,8H,1H2,2-3H3
InchiKey: YJJTXEIQRNJFQV-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: C=CC#CC(C)(C)OO
Mol. weight [g/mol]: 126.15
CAS: 14906-26-4

Physical Properties

Property code	Value	Unit	Source
chl	-4247.40 ± 1.80	kJ/mol	NIST Webbook
gf	59.72	kJ/mol	Joback Method
hf	127.10 ± 1.90	kJ/mol	NIST Webbook
hfl	63.60 ± 1.90	kJ/mol	NIST Webbook
hfus	13.59	kJ/mol	Joback Method
hvap	63.50 ± 0.20	kJ/mol	NIST Webbook
hvap	63.50	kJ/mol	NIST Webbook
log10ws	-1.91		Crippen Method
logp	1.444		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	476.61	K	Joback Method
tc	672.33	K	Joback Method
tf	358.46	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.54	J/mol×K	476.61	Joback Method
cpg	235.05	J/mol×K	509.23	Joback Method
cpg	244.07	J/mol×K	541.85	Joback Method
cpg	252.61	J/mol×K	574.47	Joback Method
cpg	260.69	J/mol×K	607.09	Joback Method
cpg	268.33	J/mol×K	639.71	Joback Method

cpg	275.56	J/mol×K	672.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14906264&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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