t-Butyldimethylvinylethynylperoxide

Inchi: InChI=1S/C11H18O2/c1-7-8-9-11(5,6)13-12-10(2,3)4/h7H,1H2,2-6H3
InchiKey: NRZBWVAKKOCBFV-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=CC#CC(C)(C)OOC(C)(C)C
Mol. weight [g/mol]: 182.26
CAS: 14906-32-2

Physical Properties

Property code	Value	Unit	Source
chl	-6872.20 ± 3.50	kJ/mol	NIST Webbook
gf	128.06	kJ/mol	Joback Method
hf	22.70 ± 3.50	kJ/mol	NIST Webbook
hfl	-28.90 ± 3.50	kJ/mol	NIST Webbook
hfus	13.64	kJ/mol	Joback Method
hvap	51.60 ± 0.20	kJ/mol	NIST Webbook
hvap	51.60	kJ/mol	NIST Webbook
log10ws	-3.46		Crippen Method
logp	2.701		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	495.14	K	Joback Method
tc	703.95	K	Joback Method
tf	367.37	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.31	J/mol×K	495.14	Joback Method
cpg	388.02	J/mol×K	529.94	Joback Method
cpg	403.79	J/mol×K	564.74	Joback Method
cpg	418.66	J/mol×K	599.55	Joback Method
cpg	432.66	J/mol×K	634.35	Joback Method
cpg	445.84	J/mol×K	669.15	Joback Method

cpg	458.22	J/mol×K	703.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14906322&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

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