1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-

Other names:	1,2,4,5-Tetraoxacyclohexane, 3,3,6,6-tetramethyl
	3,3,6,6-tetramethyl-1,2,4,5-tetroxane
	Acetone diperoxide
	DADP
	Diacetone peroxide
	Diisopropylidene cyclic diperoxide
	S-Tetroxane, 3,3,6,6-tetramethyl-
	diacetone diperoxide
Inchi:	InChI=1S/C6H12O4/c1-5(2)7-9-6(3,4)10-8-5/h1-4H3
InchiKey:	SJQITXILEOCXGI-UHFFFAOYSA-N
Formula:	C6H12O4
SMILES:	CC1(C)OOC(C)(C)OO1
Mol. weight [g/mol]:	148.16
CAS:	1073-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-339.08	kJ/mol	Joback Method
hf	-630.71	kJ/mol	Joback Method
hfus	23.52	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.369		Crippen Method
mcvol	108.020	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	860.70		NIST Webbook
rinpol	837.20		NIST Webbook
rinpol	849.80		NIST Webbook
rinpol	848.90		NIST Webbook
rinpol	861.60		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	858.90		NIST Webbook
rinpol	840.90		NIST Webbook
rinpol	849.80		NIST Webbook
rinpol	840.90		NIST Webbook
rinpol	873.60		NIST Webbook
rinpol	865.00		NIST Webbook

tb	459.84	K	Joback Method
tc	682.72	K	Joback Method
tf	406.15	K	THERMOCHEMISTRY OF CYCLIC ACETONE PEROXIDES
tf	406.15	K	A comparative study on two explosive acetone peroxides
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.59	J/mol×K	459.84	Joback Method
cpg	267.53	J/mol×K	496.99	Joback Method
cpg	280.27	J/mol×K	534.13	Joback Method
cpg	291.97	J/mol×K	571.28	Joback Method
cpg	302.83	J/mol×K	608.42	Joback Method
cpg	313.04	J/mol×K	645.57	Joback Method
cpg	322.78	J/mol×K	682.72	Joback Method

Sources

A comparative study on two explosive acetone peroxides:	https://www.doi.org/10.1016/j.tca.2013.08.009
THERMOCHEMISTRY OF CYCLIC ACETONE PEROXIDES:	https://www.doi.org/10.1016/j.tca.2014.03.046
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1073912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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