TATP

Other names:	1,2,4,5,7,8-Hexaoxacyclononane, 3,3,6,6,9,9-hexamethyl
	3,3,6,6,9,9-Hexamethyl-1,2,4,5,7,8-hexoxanane
	Acetone cyclic triperoxide
	Acetone peroxide trimer
	TATP (triacetone triperoxide)
	TCAP
	Triacetontriperoxide
	Tricycloacetonperoxide
	Trimeric acetonperoxide
	triacetone triperoxide
Inchi:	InChI=1S/C9H18O6/c1-7(2)10-12-8(3,4)14-15-9(5,6)13-11-7/h1-6H3
InchiKey:	ZTLXICJMNFREPA-UHFFFAOYSA-N
Formula:	C9H18O6
SMILES:	CC1(C)OOC(C)(C)OOC(C)(C)OO1
Mol. weight [g/mol]:	222.24
CAS:	17088-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-535.56	kJ/mol	Joback Method
hf	-980.21	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	59.56	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.053		Crippen Method
mcvol	162.030	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1128.10		NIST Webbook
rinpol	1120.60		NIST Webbook
rinpol	1122.60		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1115.30		NIST Webbook
rinpol	1125.80		NIST Webbook
rinpol	1105.80		NIST Webbook
rinpol	1111.90		NIST Webbook

rinpol	1094.00		NIST Webbook
tb	590.76	K	Joback Method
tc	831.82	K	Joback Method
tf	370.15	K	A comparative study on two explosive acetone peroxides
tf	370.15	K	THERMOCHEMISTRY OF CYCLIC ACETONE PEROXIDES
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.57	J/mol×K	590.76	Joback Method
cpg	468.30	J/mol×K	630.94	Joback Method
cpg	485.08	J/mol×K	671.11	Joback Method
cpg	501.23	J/mol×K	711.29	Joback Method
cpg	517.04	J/mol×K	751.46	Joback Method
cpg	532.84	J/mol×K	791.64	Joback Method
cpg	548.93	J/mol×K	831.82	Joback Method
psub	6.82e-03	kPa	303.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.01	kPa	308.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.02	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	0.03	kPa	318.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.05	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.07	kPa	328.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.10	kPa	333.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.12	kPa	338.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

Sources

Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034
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=C17088378&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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume