1,4-Cyclohexanedione, 2,2,6-trimethyl-

Other names:	2,6,6-Trimethyl-1,4-cyclohexanedione
	3,5,5-Trimethyl-1,4-cyclohexadione
	3,5,5-Trimethyl-1,4-cyclohexanedione
	2,2,6-Trimethyl-1,4-cyclohexanedione
	2,2,6-Trimethylcyclohexane-1,4-dione
	2,6,6-Trimethyl-1,4-cyclohexa-dione
	Cyclohexan-1,4-dione, 2,2,6-trimethyl
	Dihydrooxophorone
	1,4-cyclohexanedione-2,6,6-trimethyl
Inchi:	InChI=1S/C9H14O2/c1-6-4-7(10)5-9(2,3)8(6)11/h6H,4-5H2,1-3H3
InchiKey:	HVHHZSFNAYSPSA-UHFFFAOYSA-N
Formula:	C9H14O2
SMILES:	CC1CC(=O)CC(C)(C)C1=O
Mol. weight [g/mol]:	154.21
CAS:	20547-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-209.03	kJ/mol	Joback Method
hf	-455.27	kJ/mol	Joback Method
hfus	4.69	kJ/mol	Joback Method
hvap	43.09	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.581		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1168.50		NIST Webbook
rinpol	1170.30		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1196.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1782.00		NIST Webbook

tb	556.08	K	Joback Method
tc	798.51	K	Joback Method
tf	354.67	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.74	J/mol×K	556.08	Joback Method
cpg	341.55	J/mol×K	596.48	Joback Method
cpg	358.48	J/mol×K	636.89	Joback Method
cpg	374.59	J/mol×K	677.29	Joback Method
cpg	389.95	J/mol×K	717.70	Joback Method
cpg	404.60	J/mol×K	758.10	Joback Method
cpg	418.61	J/mol×K	798.51	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20547993&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume