1,3-Cyclobutanedione, 2,2,4,4-tetramethyl-

Other names:	Tetramethyl-1,3-cyclobutanedione
	Tetramethylcyclobuta-1,3-dione
	1,1,3,3-Tetramethylcyclobutanedione
	2,2,4,4-Tetramethyl-1,3-cyclobutanedione
	2,2,4,4-Tetramethylcyclobutanedione
	2,2,4,4-Tetramethyl cyclobutane-1,3-dione
	tetramethylcyclobutane-1,3-dione
Inchi:	InChI=1S/C8H12O2/c1-7(2)5(9)8(3,4)6(7)10/h1-4H3
InchiKey:	RGCDVHNITQEYPO-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC1(C)C(=O)C(C)(C)C1=O
Mol. weight [g/mol]:	140.18
CAS:	933-52-8

Physical Properties

Property code	Value	Unit	Source
chs	-4483.20 ± 1.40	kJ/mol	NIST Webbook
gf	-198.74	kJ/mol	Joback Method
hf	-307.70 ± 1.60	kJ/mol	NIST Webbook
hfs	-379.90 ± 1.50	kJ/mol	NIST Webbook
hfus	0.01	kJ/mol	Joback Method
hsub	72.20 ± 0.60	kJ/mol	NIST Webbook
hvap	39.37	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.00 ± 0.02	eV	NIST Webbook
log10ws	-1.14		Crippen Method
logp	1.191		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	524.90	K	Joback Method
tc	764.54	K	Joback Method
tf	374.34	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.66	J/mol×K	524.90	Joback Method
cpg	291.07	J/mol×K	564.84	Joback Method
cpg	304.62	J/mol×K	604.78	Joback Method
cpg	317.51	J/mol×K	644.72	Joback Method
cpg	329.93	J/mol×K	684.66	Joback Method
cpg	342.06	J/mol×K	724.60	Joback Method
cpg	354.08	J/mol×K	764.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.20	K	100.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C933528&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume