Cyclobutanone, 2,2,3-trimethyl-

Other names: 2,2,3-Trimethylcyclobutanone
Inchi: InChI=1S/C7H12O/c1-5-4-6(8)7(5,2)3/h5H,4H2,1-3H3
InchiKey: XCNUTNIUANPMKW-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC1CC(=O)C1(C)C
Mol. weight [g/mol]: 112.17
CAS: 1449-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-79.08	kJ/mol	Joback Method
hf	-263.97	kJ/mol	Joback Method
hfus	4.20	kJ/mol	Joback Method
hvap	34.05	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.621		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	787.00		NIST Webbook
tb	433.96	K	Joback Method
tc	649.38	K	Joback Method
tf	270.95	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.76	J/mol×K	433.96	Joback Method
cpg	222.10	J/mol×K	469.86	Joback Method
cpg	235.56	J/mol×K	505.77	Joback Method
cpg	248.22	J/mol×K	541.67	Joback Method
cpg	260.16	J/mol×K	577.57	Joback Method
cpg	271.46	J/mol×K	613.47	Joback Method
cpg	282.21	J/mol×K	649.38	Joback Method

Sources

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=C1449496&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