Cyclopentanone, 2,2,4-trimethyl-

Other names:	2,2,4-Trimethylcyclopentanone
	2,2,4-trimethylcyclopentan-1-one
Inchi:	InChI=1S/C8H14O/c1-6-4-7(9)8(2,3)5-6/h6H,4-5H2,1-3H3
InchiKey:	PJXIBUIXCXSNCM-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC1CC(=O)C(C)(C)C1
Mol. weight [g/mol]:	126.20
CAS:	28056-54-4

Physical Properties

Property code	Value	Unit	Source
gf	-82.76	kJ/mol	Joback Method
hf	-290.77	kJ/mol	Joback Method
hfus	4.69	kJ/mol	Joback Method
hvap	36.45	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	461.11	K	Joback Method
tc	682.24	K	Joback Method
tf	278.70	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.57	J/mol×K	461.11	Joback Method
cpg	265.00	J/mol×K	497.96	Joback Method
cpg	280.47	J/mol×K	534.82	Joback Method
cpg	295.06	J/mol×K	571.67	Joback Method
cpg	308.86	J/mol×K	608.53	Joback Method
cpg	321.95	J/mol×K	645.38	Joback Method
cpg	334.42	J/mol×K	682.24	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=C28056544&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume