Cyclopentanone, 2-methyl-3-(1-methylethyl)-

Other names: «beta»-Thujamenthone
Inchi: InChI=1S/C9H16O/c1-6(2)8-4-5-9(10)7(8)3/h6-8H,4-5H2,1-3H3
InchiKey: VWBCFESGRRREEF-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC(C)C1CCC(=O)C1C
Mol. weight [g/mol]: 140.22
CAS: 54549-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-71.29	kJ/mol	Joback Method
hf	-331.93	kJ/mol	Joback Method
hfus	10.06	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.258		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	483.31	K	Joback Method
tc	696.81	K	Joback Method
tf	251.07	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.27	J/mol×K	483.31	Joback Method
cpg	310.04	J/mol×K	518.89	Joback Method
cpg	327.03	J/mol×K	554.48	Joback Method
cpg	343.24	J/mol×K	590.06	Joback Method
cpg	358.67	J/mol×K	625.64	Joback Method
cpg	373.31	J/mol×K	661.23	Joback Method

cpg	387.18	J/mol×K	696.81	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=C54549814&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume