(R)-(+)-3-Methylcyclopentanone

Other names: Cyclopentanone, 3-methyl-, (R)-
(+)-3-methylcyclopentanone
Inchi: InChI=1S/C6H10O/c1-5-2-3-6(7)4-5/h5H,2-4H2,1H3/t5-/m0/s1
InchiKey: AOKRXIIIYJGNNU-YFKPBYRVSA-N
Formula: C6H10O
SMILES: CC1CCC(=O)C1
Mol. weight [g/mol]: 98.14
CAS: 6672-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-86.40	kJ/mol	Joback Method
hf	-244.39	kJ/mol	Joback Method
hfus	4.74	kJ/mol	Joback Method
hvap	33.45	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.375		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	847.60		NIST Webbook
rinpol	847.60		NIST Webbook
tb	416.70	K	NIST Webbook
tc	637.42	K	Joback Method
tf	236.50	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.13	J/mol×K	419.78	Joback Method
cpg	178.43	J/mol×K	456.05	Joback Method
cpg	191.20	J/mol×K	492.33	Joback Method
cpg	203.42	J/mol×K	528.60	Joback Method
cpg	215.09	J/mol×K	564.87	Joback Method

cpg	226.22	J/mol×K	601.15	Joback Method
cpg	236.80	J/mol×K	637.42	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=C6672306&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