Cycloheptanone, 4-methyl-, (R)-

Other names: Cycloheptanone, 4-methyl-, (-)-
Inchi: InChI=1S/C8H14O/c1-7-3-2-4-8(9)6-5-7/h7H,2-6H2,1H3/t7-/m0/s1
InchiKey: WXVNSHRGPVHBPD-ZETCQYMHSA-N
Formula: C8H14O
SMILES: CC1CCCC(=O)CC1
Mol. weight [g/mol]: 126.20
CAS: 13609-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.76	kJ/mol	Joback Method
hf	-297.99	kJ/mol	Joback Method
hfus	5.72	kJ/mol	Joback Method
hvap	38.25	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	474.08	K	Joback Method
tc	703.31	K	Joback Method
tf	252.00	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.33	J/mol×K	474.08	Joback Method
cpg	264.39	J/mol×K	512.28	Joback Method
cpg	281.64	J/mol×K	550.49	Joback Method
cpg	298.06	J/mol×K	588.69	Joback Method
cpg	313.64	J/mol×K	626.90	Joback Method
cpg	328.36	J/mol×K	665.10	Joback Method
cpg	342.21	J/mol×K	703.31	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=C13609591&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