trans-3,5-Dimethylcyclohexanone

Other names: 3,5-Dimethylcyclohexanone, (E)-
Inchi: InChI=1S/C8H14O/c1-6-3-7(2)5-8(9)4-6/h6-7H,3-5H2,1-2H3/t6-,7+
InchiKey: MSANHHHQJYQEOK-KNVOCYPGSA-N
Formula: C8H14O
SMILES: CC1CC(=O)CC(C)C1
Mol. weight [g/mol]: 126.20
CAS: 7214-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-89.37	kJ/mol	Joback Method
hf	-312.17	kJ/mol	Joback Method
hfus	8.89	kJ/mol	Joback Method
hvap	37.77	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	465.14	K	Joback Method
tc	685.24	K	Joback Method
tf	251.28	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.31	J/mol×K	465.14	Joback Method
cpg	264.59	J/mol×K	501.82	Joback Method
cpg	281.16	J/mol×K	538.51	Joback Method
cpg	297.01	J/mol×K	575.19	Joback Method
cpg	312.11	J/mol×K	611.88	Joback Method
cpg	326.46	J/mol×K	648.56	Joback Method
cpg	340.04	J/mol×K	685.24	Joback Method

Sources

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=C7214495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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