3,4-Dimethylcyclohexanone

Other names: 3,4-Dimethylcyclohexanone,c&t
Cyclohexanone, 3,4-dimethyl-
Inchi: InChI=1S/C8H14O/c1-6-3-4-8(9)5-7(6)2/h6-7H,3-5H2,1-2H3
InchiKey: ZDCYWXYPRPCJOY-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CC1CCC(=O)CC1C
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
hfus	8.89	kJ/mol	Joback Method
ie	9.30	eV	Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
tb	460.00 ± 3.00	K	NIST Webbook
tf	256.39	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5465098&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point