

2,5-DIMETHYLCYCLOHEXANONE

Other names:	2,5-Dimethylcyclohexanone,c&t
Inchi:	InChI=1S/C8H14O/c1-6-3-4-7(2)8(9)5-6/h6-7H,3-5H2,1-2H3
InchiKey:	LUGFNAYTNQMMMY-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC1CCC(C)C(=O)C1
Mol. weight [g/mol]:	126.20

Physical Properties

Property code	Value	Unit	Source
hfus	8.89	kJ/mol	Joback Method
hvap	47.30	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
tb	447.00 ± 5.00	K	NIST Webbook
tf	275.58	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

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932514&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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