2,6-Dimethylcyclohexanone

Other names:	2,6-Dimethylcyclohexanone cis + trans
	2,6-Dimethylcyclohexanone,c&t
	2,6-dimethylcyclohexan-1-one
Inchi:	InChI=1S/C8H14O/c1-6-4-3-5-7(2)8(6)9/h6-7H,3-5H2,1-2H3
InchiKey:	AILVYPLQKCQNJC-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC1CCCC(C)C1=O
Mol. weight [g/mol]:	126.20
CAS:	2816-57-1

Physical Properties

Property code	Value	Unit	Source
af	0.3339		Cheméo Relay (1.0)
chl	-4765.60	kJ/mol	NIST Webbook
gf	-89.37	kJ/mol	Joback Method
hf	-276.21	kJ/mol	Cheméo Relay (1.0)
hfus	8.89	kJ/mol	Joback Method
hvap	47.31	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-1.29		Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	985.00		NIST Webbook
ripol	1322.00		NIST Webbook
tb	448.20	K	NIST Webbook
tc	649.43	K	Cheméo Relay (1.0)
tf	273.28	K	Cheméo Relay (1.0)
vc	0.390	m3/kmol	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44348e+01
Coeff. B	-3.75444e+03
Coeff. C	-6.57360e+01
Temperature range (K), min.	331.12
Temperature range (K), max.	477.26

Sources

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2816571&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume