2-Cyclohexen-1-one, 4,4-dimethyl-

Other names: 4,4-Dimethyl-2-cyclohexen-1-one
4,4-Dimethyl-2-cyclohexenone
4,4-Dimethylcyclohexenone
Inchi: InChI=1S/C8H12O/c1-8(2)5-3-7(9)4-6-8/h3,5H,4,6H2,1-2H3
InchiKey: HAUNPYVLVAIUOO-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1(C)C=CC(=O)CC1
Mol. weight [g/mol]: 124.18
CAS: 1073-13-8

Physical Properties

Property code	Value	Unit	Source
gf	-57.19	kJ/mol	Joback Method
hf	-218.81	kJ/mol	Joback Method
hfus	2.75	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
ripol	1651.00		NIST Webbook
tb	469.21	K	Joback Method
tc	702.04	K	Joback Method
tf	280.18	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.71	J/mol×K	469.21	Joback Method
cpg	247.44	J/mol×K	508.02	Joback Method
cpg	262.16	J/mol×K	546.82	Joback Method
cpg	275.96	J/mol×K	585.63	Joback Method
cpg	288.94	J/mol×K	624.43	Joback Method

cpg	301.21	J/mol×K	663.24	Joback Method
cpg	312.85	J/mol×K	702.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.00	K	2.70	NIST Webbook

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=C1073138&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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