2-Cyclohexen-1-one, 3,5-dimethyl-

Other names: 3,5-Dimethyl-2-cyclohexen-1-one
3,5-Dimethyl-2-cyclohexene-1-one
3,5-dimethylcyclohex-2-en-1-one
Inchi: InChI=1S/C8H12O/c1-6-3-7(2)5-8(9)4-6/h4,7H,3,5H2,1-2H3
InchiKey: NOQKKFBBAODEHN-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1=CC(=O)CC(C)C1
Mol. weight [g/mol]: 124.18
CAS: 1123-09-7

Physical Properties

Property code	Value	Unit	Source
chl	-4648.80	kJ/mol	NIST Webbook
gf	-61.33	kJ/mol	Joback Method
hf	-245.52	kJ/mol	Joback Method
hfus	8.65	kJ/mol	Joback Method
hvap	39.03	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
ripol	1624.00		NIST Webbook
ripol	1597.00		NIST Webbook
tb	484.70	K	NIST Webbook
tc	697.99	K	Joback Method
tf	268.80	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.75	J/mol×K	473.95	Joback Method
cpg	246.94	J/mol×K	511.29	Joback Method
cpg	261.49	J/mol×K	548.63	Joback Method

cpg	275.38	J/mol×K	585.97	Joback Method
cpg	288.61	J/mol×K	623.31	Joback Method
cpg	301.16	J/mol×K	660.65	Joback Method
cpg	313.01	J/mol×K	697.99	Joback Method

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=C1123097&Units=SI

Legend

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume