2-Propanone, 1-(dimethylamino)-

Other names: (Dimethylamino)acetone
N,N-Dimethylaminoacetone
1-(Dimethylamino)-2-propanone
1-Dimethylaminoacetone
(CH3)2NCH2COCH3
Inchi: InChI=1S/C5H11NO/c1-5(7)4-6(2)3/h4H2,1-3H3
InchiKey: VFPKIWATTACVJR-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CC(=O)CN(C)C
Mol. weight [g/mol]: 101.15
CAS: 15364-56-4

Physical Properties

Property code	Value	Unit	Source
chl	-3315.90 ± 2.90	kJ/mol	NIST Webbook
gf	-26.92	kJ/mol	Joback Method
hf	-180.10 ± 2.90	kJ/mol	NIST Webbook
hfl	-223.70 ± 2.90	kJ/mol	NIST Webbook
hfus	13.33	kJ/mol	Joback Method
hvap	43.60 ± 0.30	kJ/mol	NIST Webbook
hvap	43.60 ± 0.25	kJ/mol	NIST Webbook
ie	7.71 ± 0.03	eV	NIST Webbook
ie	7.71 ± 0.05	eV	NIST Webbook
ie	8.65	eV	NIST Webbook
log10ws	0.23		Crippen Method
logp	0.137		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	712.00		NIST Webbook
rinpol	712.00		NIST Webbook
tb	392.70	K	NIST Webbook
tc	556.89	K	Joback Method
tf	228.51	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.27	J/mol×K	380.11	Joback Method
cpg	178.30	J/mol×K	409.57	Joback Method
cpg	187.90	J/mol×K	439.04	Joback Method
cpg	197.08	J/mol×K	468.50	Joback Method
cpg	205.86	J/mol×K	497.96	Joback Method
cpg	214.24	J/mol×K	527.43	Joback Method
cpg	222.23	J/mol×K	556.89	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=C15364564&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
hfl: Liquid phase 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume