

Ethanone, 2-(dimethylamino)-1-phenyl-

Other names:	Acetophenone, 2-(dimethylamino)- «alpha»-(Dimethylamino)acetophenone [(Dimethylamino)acetyl]benzene 2-(Dimethylamino)acetophenone
Inchi:	InChI=1S/C10H13NO/c1-11(2)8-10(12)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey:	UMLWXYJZDNNBTD-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CN(C)CC(=O)c1ccccc1
Mol. weight [g/mol]:	163.22
CAS:	3319-03-7

Physical Properties

Property code	Value	Unit	Source
chl	-5676.99 ± 0.93	kJ/mol	NIST Webbook
gf	127.59	kJ/mol	Joback Method
hf	-46.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-116.00 ± 0.98	kJ/mol	NIST Webbook
hfus	20.32	kJ/mol	Joback Method
hvap	69.66 ± 0.54	kJ/mol	NIST Webbook
hvap	69.70 ± 0.50	kJ/mol	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.431		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	521.19	K	Joback Method
tc	732.99	K	Joback Method
tf	311.28	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.15	J/mol×K	521.19	Joback Method
cpg	324.85	J/mol×K	556.49	Joback Method

cpg	338.60	J/mol×K	591.79	Joback Method
cpg	351.47	J/mol×K	627.09	Joback Method
cpg	363.49	J/mol×K	662.39	Joback Method
cpg	374.69	J/mol×K	697.69	Joback Method
cpg	385.14	J/mol×K	732.99	Joback Method

Sources

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=C3319037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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