4-N,N-Dimethylaminoacetophenone

Other names:	p-Dimethylaminoacetophenone p-N,N-Dimethylaminoacetophenone Acetophenone, 4'-(dimethylamino)- Ethanone, 1-(4-(dimethylamino)phenyl)- 4-Dimethylaminoacetophenone 4'-(Dimethylamino)acetophenone
Inchi:	InChI=1S/C10H13NO/c1-8(12)9-4-6-10(7-5-9)11(2)3/h4-7H,1-3H3
InchiKey:	HUDYANRNMZDQGA-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CC(=O)c1ccc(N(C)C)cc1
Mol. weight [g/mol]:	163.22
CAS:	2124-31-4

Physical Properties

Property code	Value	Unit	Source
affp	932.80	kJ/mol	NIST Webbook
basg	906.30	kJ/mol	NIST Webbook
gf	117.96	kJ/mol	Joback Method
hf	-69.72	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
ie	7.57 ± 0.05	eV	NIST Webbook
ie	7.55	eV	NIST Webbook
ie	7.69	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.955		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	526.17	K	Joback Method
tc	739.11	K	Joback Method
tf	323.80	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.22	J/mol×K	526.17	Joback Method
cpg	324.55	J/mol×K	561.66	Joback Method
cpg	338.00	J/mol×K	597.15	Joback Method
cpg	350.61	J/mol×K	632.64	Joback Method
cpg	362.42	J/mol×K	668.13	Joback Method
cpg	373.47	J/mol×K	703.62	Joback Method
cpg	383.78	J/mol×K	739.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2124314&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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