

Benzophenone, 2-methylamino-5-chloro-

Other names:	Methanone, [2-(aminomethyl)-5-chlorophenyl]phenyl-
Inchi:	InChI=1S/C14H12ClNO/c15-12-7-6-11(9-16)13(8-12)14(17)10-4-2-1-3-5-10/h1-8H,9,16H
InchiKey:	YHSCBLSYYDIOFJ-UHFFFAOYSA-N
Formula:	C14H12ClNO
SMILES:	NCc1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]:	245.70
CAS:	74966-83-9

Physical Properties

Property code	Value	Unit	Source
gf	198.16	kJ/mol	Joback Method
hf	23.30	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	74.41	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.030		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	746.87	K	Joback Method
tc	1002.53	K	Joback Method
tf	488.53	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.61	J/molxK	746.87	Joback Method
cpg	483.47	J/molxK	789.48	Joback Method
cpg	495.18	J/molxK	832.09	Joback Method
cpg	505.83	J/molxK	874.70	Joback Method

cpg	515.50	J/mol×K	917.31	Joback Method
cpg	524.25	J/mol×K	959.92	Joback Method
cpg	532.18	J/mol×K	1002.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C74966839&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
mvol:	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

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