3-Aminobenzophenone

Other names: Methanone, (3-aminophenyl)phenyl-
Benzophenone, 3-amino-
m-Aminobenzophenone
3-Benzoylaniline
Inchi: InChI=1S/C13H11NO/c14-12-8-4-7-11(9-12)13(15)10-5-2-1-3-6-10/h1-9H,14H2
InchiKey: FUADXEJBHCKVBN-UHFFFAOYSA-N
Formula: C13H11NO
SMILES: Nc1cccc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 197.23
CAS: 2835-78-1

Physical Properties

Property code	Value	Unit	Source
gf	211.30	kJ/mol	Joback Method
hf	71.15	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	67.13	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-3.06		Crippen Method
logp	2.500		Crippen Method
mcvol	158.060	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	681.58	K	Joback Method
tc	940.51	K	Joback Method
tf	434.82	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.28	J/mol×K	681.58	Joback Method
cpg	412.12	J/mol×K	724.73	Joback Method
cpg	424.72	J/mol×K	767.89	Joback Method

cpg	436.18	J/mol×K	811.04	Joback Method
cpg	446.58	J/mol×K	854.20	Joback Method
cpg	455.99	J/mol×K	897.35	Joback Method
cpg	464.50	J/mol×K	940.51	Joback Method

Sources

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=C2835781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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