Benzophenone, 2-amino-5-chloro-

Other names:	Methanone, (2-amino-5-chlorophenyl)phenyl-
	2-Amino-5-chlorbenzophenone
	2-Amino-5-chlorobenzophenone
	2-Benzoyl-4-chloroaniline
	5-Chloro-2-aminobenzophenone
	(2-Amino-5-chlorophenyl)phenylmethanone
	2-Amino-5-chlorbenzophenon
	2-Amino-5-chlorobenzylphenone
	NSC 84157
	Oxazepam benzophenone
	Chlordiazepoxide benzophenone
Inchi:	InChI=1S/C13H10ClNO/c14-10-6-7-12(15)11(8-10)13(16)9-4-2-1-3-5-9/h1-8H,15H2
InchiKey:	ZUWXHHBROGLWNH-UHFFFAOYSA-N
Formula:	C13H10ClNO
SMILES:	Nc1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]:	231.68
CAS:	719-59-5

Physical Properties

Property code	Value	Unit	Source
gf	189.74	kJ/mol	Joback Method
hf	43.94	kJ/mol	Joback Method
hfus	27.72	kJ/mol	Joback Method
hvap	72.18	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.153		Crippen Method
mcvol	170.300	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2005.00		NIST Webbook

rinpol	1994.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2028.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	723.99	K	Joback Method
tc	985.70	K	Joback Method
tf	477.26	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.34	J/mol×K	723.99	Joback Method
cpg	431.67	J/mol×K	767.61	Joback Method
cpg	442.87	J/mol×K	811.23	Joback Method
cpg	453.01	J/mol×K	854.84	Joback Method
cpg	462.18	J/mol×K	898.46	Joback Method
cpg	470.44	J/mol×K	942.08	Joback Method
cpg	477.87	J/mol×K	985.70	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=C719595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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