Methanone, (2-amino-5-chlorophenyl)(2-chlorophenyl)-

Other names: 2-Amino-2',5-dichlorobenzophenone
Benzophenone, 2-amino-2',5-dichloro-
2-Amino-5,2'-dichlor-benzophenone
2-Amino-5,2'-dichlorobenzophenone

Inchi: InChI=1S/C13H9Cl2NO/c14-8-5-6-12(16)10(7-8)13(17)9-3-1-2-4-11(9)15/h1-7H,16H2

InchiKey: KWZYIAJRFJVQDO-UHFFFAOYSA-N

Formula: C13H9Cl2NO

SMILES: Nc1ccc(Cl)cc1C(=O)c1ccccc1Cl

Mol. weight [g/mol]: 266.12

CAS: 2958-36-3

Physical Properties

Property code	Value	Unit	Source
gf	168.18	kJ/mol	Joback Method
hf	16.73	kJ/mol	Joback Method
hfus	31.53	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.807		Crippen Method
mcvol	182.540	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	2145.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	766.40	K	Joback Method
tc	1030.46	K	Joback Method
tf	519.70	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	438.38	J/mol×K	766.40	Joback Method
cpg	449.32	J/mol×K	810.41	Joback Method
cpg	459.21	J/mol×K	854.42	Joback Method
cpg	468.13	J/mol×K	898.43	Joback Method
cpg	476.14	J/mol×K	942.44	Joback Method
cpg	483.32	J/mol×K	986.45	Joback Method
cpg	489.73	J/mol×K	1030.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2958363&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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