Benzophenone, 2,5-diamino-2'-chloro-

Other names: Benzophenone, 2'-chloro-2,5-diamino
Inchi: InChI=1S/C13H11ClN2O/c14-11-4-2-1-3-9(11)13(17)10-7-8(15)5-6-12(10)16/h1-7H,15-1
InchiKey: HMTGFGCXWOUKTO-UHFFFAOYSA-N
Formula: C13H11ClN2O
SMILES: Nc1ccc(N)c(C(=O)c2ccccc2Cl)c1
Mol. weight [g/mol]: 246.69
CAS: 58479-51-9

Physical Properties

Property code	Value	Unit	Source
gf	246.56	kJ/mol	Joback Method
hf	66.26	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	83.48	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.735		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	801.50	K	Joback Method
tc	1067.22	K	Joback Method
tf	573.04	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.21	J/mol×K	801.50	Joback Method
cpg	482.31	J/mol×K	845.79	Joback Method
cpg	492.34	J/mol×K	890.07	Joback Method
cpg	501.37	J/mol×K	934.36	Joback Method

cpg	509.47	J/mol×K	978.65	Joback Method
cpg	516.72	J/mol×K	1022.94	Joback Method
cpg	523.20	J/mol×K	1067.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58479519&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