2-amino-3-hydroxy-5-chloro-benzophenone

Other names: Benzophenone, 2-amino-5-chloro-3-hydroxy
Inchi: InChI=1S/C13H10ClNO2/c14-9-6-10(12(15)11(16)7-9)13(17)8-4-2-1-3-5-8/h1-7,16H,15H
InchiKey: XJFFXSCDIWNOAH-UHFFFAOYSA-N
Formula: C13H10ClNO2
SMILES: Nc1c(O)cc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]: 247.68

Physical Properties

Property code	Value	Unit	Source
gf	35.12	kJ/mol	Joback Method
hf	-133.37	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	85.19	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.859		Crippen Method
mcvol	176.170	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2382.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	804.61	K	Joback Method
tc	1071.58	K	Joback Method
tf	588.98	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.08	J/mol×K	804.61	Joback Method
cpg	470.74	J/mol×K	849.11	Joback Method
cpg	480.70	J/mol×K	893.60	Joback Method
cpg	490.10	J/mol×K	938.10	Joback Method

cpg	499.11	J/mol×K	982.59	Joback Method
cpg	507.87	J/mol×K	1027.09	Joback Method
cpg	516.54	J/mol×K	1071.58	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=R17547&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