5-Amino-2-hydroxy-4-methoxy benzophenone

Inchi: InChI=1S/C14H13NO3/c1-18-13-8-12(16)10(7-11(13)15)14(17)9-5-3-2-4-6-9/h2-8,16H,1
InchiKey: CYJDNZBDFFCQOZ-UHFFFAOYSA-N
Formula: C14H13NO3
SMILES: COc1cc(O)c(C(=O)c2ccccc2)cc1N
Mol. weight [g/mol]: 243.26
CAS: 116495-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-49.53	kJ/mol	Joback Method
hf	-270.49	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	85.45	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.214		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	812.48	K	Joback Method
tc	1067.76	K	Joback Method
tf	592.56	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.05	J/mol×K	812.48	Joback Method
cpg	529.05	J/mol×K	855.03	Joback Method
cpg	540.22	J/mol×K	897.57	Joback Method
cpg	550.67	J/mol×K	940.12	Joback Method
cpg	560.52	J/mol×K	982.67	Joback Method
cpg	569.86	J/mol×K	1025.21	Joback Method
cpg	578.82	J/mol×K	1067.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495864&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume