5-Amino-2'-fluoro-2-methylaminobenzophenone

Other names: 2-methylamino-5-amino-2'-fluoro-benzophenone
Benzophenone, 5-amino-2'-fluoro-2-methylamino
Inchi: InChI=1S/C14H13FN2O/c1-17-13-7-6-9(16)8-11(13)14(18)10-4-2-3-5-12(10)15/h2-8,17H
InchiKey: JPJCSZZRWRMPRU-UHFFFAOYSA-N
Formula: C14H13FN2O
SMILES: CNc1ccc(N)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]: 244.26
CAS: 67739-73-5

Physical Properties

Property code	Value	Unit	Source
gf	95.04	kJ/mol	Joback Method
hf	-115.07	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.681		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
rinpol	2700.00		NIST Webbook
rinpol	2703.00		NIST Webbook
tb	763.86	K	Joback Method
tc	1003.99	K	Joback Method
tf	524.38	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.92	J/mol×K	763.86	Joback Method
cpg	516.55	J/mol×K	803.88	Joback Method
cpg	528.14	J/mol×K	843.90	Joback Method

cpg	538.73	J/mol×K	883.92	Joback Method
cpg	548.39	J/mol×K	923.94	Joback Method
cpg	557.17	J/mol×K	963.97	Joback Method
cpg	565.14	J/mol×K	1003.99	Joback Method

Sources

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=C67739735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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