2-Amino-5-bromo-2'-fluorobenzophenone

Other names: 2-Amino-2'-fluoro-5-bromobenzophenone
Methanone, (2-amino-5-bromophenyl)(2-fluorophenyl)-
Inchi: InChI=1S/C13H9BrFNO/c14-8-5-6-12(16)10(7-8)13(17)9-3-1-2-4-11(9)15/h1-7H,16H2
InchiKey: XCOKDXNGCQXFCV-UHFFFAOYSA-N
Formula: C13H9BrFNO
SMILES: Nc1ccc(Br)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]: 294.12
CAS: 1479-58-9

Physical Properties

Property code	Value	Unit	Source
gf	11.55	kJ/mol	Joback Method
hf	-121.57	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.401		Crippen Method
mcvol	177.330	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	756.97	K	Joback Method
tc	1015.29	K	Joback Method
tf	520.25	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.43	J/mol×K	756.97	Joback Method
cpg	445.49	J/mol×K	800.02	Joback Method
cpg	455.54	J/mol×K	843.08	Joback Method
cpg	464.68	J/mol×K	886.13	Joback Method

cpg	472.97	J/mol×K	929.18	Joback Method
cpg	480.49	J/mol×K	972.24	Joback Method
cpg	487.32	J/mol×K	1015.29	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=C1479589&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume