Methanone, (2-amino-5-chlorophenyl)(2-fluorophenyl)-

Other names: 2-Amino-2'-fluoro-5-chlorobenzophenone
2-Amino-5-chloro-2'-fluorobenzophenone
Benzophenone, 2-amino-5-chloro-2'-fluoro-
2-amino-5-chlor-2'-fluor-benzophenone

Inchi: InChI=1S/C13H9ClFNO/c14-8-5-6-12(16)10(7-8)13(17)9-3-1-2-4-11(9)15/h1-7H,16H2

InchiKey: GTGMXPIQRQSORU-UHFFFAOYSA-N

Formula: C13H9ClFNO

SMILES: Nc1ccc(Cl)cc1C(=O)c1ccccc1F

Mol. weight [g/mol]: 249.67

CAS: 784-38-3

Physical Properties

Property code	Value	Unit	Source
gf	-14.70	kJ/mol	Joback Method
hf	-163.64	kJ/mol	Joback Method
hfus	30.41	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.292		Crippen Method
mcvol	172.070	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	728.24	K	Joback Method
tc	978.73	K	Joback Method
tf	490.37	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.65	J/mol×K	728.24	Joback Method

cpg	437.19	J/mol×K	769.99	Joback Method
cpg	447.71	J/mol×K	811.74	Joback Method
cpg	457.28	J/mol×K	853.48	Joback Method
cpg	465.95	J/mol×K	895.23	Joback Method
cpg	473.79	J/mol×K	936.98	Joback Method
cpg	480.85	J/mol×K	978.73	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=C784383&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