2-Methylamino-5-chloro-2'-fluorobenzophenone

Inchi: InChI=1S/C14H11ClFNO/c1-17-13-7-6-9(15)8-11(13)14(18)10-4-2-3-5-12(10)16/h2-8,17
InchiKey: ULELQOJFPCDNFG-UHFFFAOYSA-N
Formula: C14H11ClFNO
SMILES: CNc1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]: 263.69

Physical Properties

Property code	Value	Unit	Source
gf	16.66	kJ/mol	Joback Method
hf	-164.60	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	70.05	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.752		Crippen Method
mcvol	186.160	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	728.76	K	Joback Method
tc	966.39	K	Joback Method
tf	471.04	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.61	J/mol×K	728.76	Joback Method
cpg	482.13	J/mol×K	768.36	Joback Method
cpg	493.62	J/mol×K	807.97	Joback Method
cpg	504.15	J/mol×K	847.57	Joback Method
cpg	513.77	J/mol×K	887.18	Joback Method
cpg	522.54	J/mol×K	926.78	Joback Method
cpg	530.51	J/mol×K	966.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66764&Units=SI
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

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

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