

2-amino-5-chloro-2'-fluorobenzophenone, acetylated

Inchi: InChI=1S/C15H11ClFNO2/c1-9(19)18-14-7-6-10(16)8-12(14)15(20)11-4-2-3-5-13(11)17//
InchiKey: BIJCUDKFSIRCDI-UHFFFAOYSA-N
Formula: C15H11ClFNO2
SMILES: CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccccc1F
Mol. weight [g/mol]: 291.71

Physical Properties

Property code	Value	Unit	Source
hfus	37.09	kJ/mol	Joback Method
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-4.28		Cheméo Relay (1.0)
logp	3.669		Crippen Method
mcvol	201.820	ml/mol	McGowan Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	634.33	K	Cheméo Relay (1.0)
tf	387.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.69	J/mol×K	805.51	Joback Method
cpg	542.86	J/mol×K	845.23	Joback Method
cpg	553.02	J/mol×K	884.95	Joback Method
cpg	562.23	J/mol×K	924.67	Joback Method
cpg	570.55	J/mol×K	964.39	Joback Method
cpg	578.03	J/mol×K	1004.10	Joback Method
cpg	584.72	J/mol×K	1043.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313005&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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