Acetophenone, 2'-amino, PFBO # 2

Inchi: InChI=1S/C15H11F5N2O/c1-7(8-4-2-3-5-10(8)21)22-23-6-9-11(16)13(18)15(20)14(19)12

InchiKey: IMEZFULKLNMRHL-UHFFFAOYSA-N

Formula: C15H11F5N2O

SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)c1ccccc1N

Mol. weight [g/mol]: 330.25

Physical Properties

Property code	Value	Unit	Source
hf	-955.24	kJ/mol	Joback Method
hvap	69.87	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.905		Crippen Method
mcvol	205.070	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
ripol	2918.00		NIST Webbook
ripol	2918.00		NIST Webbook
tb	793.70	K	Joback Method
tc	1006.70	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R575154&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

Legend

hf:	Enthalpy of formation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature