Benzeneethanamine, N-[(pentafluorophenyl)methylene]-

Other names: Phenethylamine, N-(2,3,4,5,6-pentafluorobenzylidene)-
Pentafluorobenzaldehyde N-(phenethyl)imine
2-Phenylethylamine, PFB-imine

Inchi: InChI=1S/C15H10F5N/c16-11-10(12(17)14(19)15(20)13(11)18)8-21-7-6-9-4-2-1-3-5-9/h1

InchiKey: BXRZDFUZOZNVLT-UHFFFAOYSA-N

Formula: C15H10F5N

SMILES: Fc1c(F)c(F)c(C=NCCc2ccccc2)c(F)c1F

Mol. weight [g/mol]: 299.24

CAS: 29723-34-0

Physical Properties

Property code	Value	Unit	Source
hf	-835.55	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.044		Crippen Method
mcvol	189.220	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	1681.00		NIST Webbook
tb	693.89	K	Joback Method
tc	897.85	K	Joback Method

Sources

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=C29723340&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature