

Imidazolidine,2-(pentafluorophenylimino)-)

Inchi:	InChI=1S/C9H6F5N3/c10-3-4(11)6(13)8(7(14)5(3)12)17-9-15-1-2-16-9/h1-2H2,(H2,15,16)
InchiKey:	DWPNQRNRVKWYRZ-UHFFFAOYSA-N
Formula:	C9H6F5N3
SMILES:	Fc1c(F)c(F)c(N=C2NCCN2)c(F)c1F
Mol. weight [g/mol]:	251.16
CAS:	74395-26-9

Physical Properties

Property code	Value	Unit	Source
hf	-832.99	kJ/mol	Joback Method
hvap	55.35	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	1.562		Crippen Method
mcvol	137.540	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	649.46	K	Joback Method
tc	864.13	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=C74395269&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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