

2,3-Dicyanodibenzo(f,h)quinoxaline

Other names:	Dibenzo[f,h]quinoxaline-2,3-dicarbonitrile
Inchi:	InChI=1S/C18H8N4/c19-9-15-16(10-20)22-18-14-8-4-2-6-12(14)11-5-1-3-7-13(11)17(18)
InchiKey:	XAFVICNFTRNVKE-UHFFFAOYSA-N
Formula:	C18H8N4
SMILES:	N#Cc1nc2c3ccccc3c3ccccc3c2nc1C#N
Mol. weight [g/mol]:	280.28
CAS:	55408-49-6

Physical Properties

Property code	Value	Unit	Source
ie	8.20	eV	NIST Webbook
log10ws	-7.12		Crippen Method
logp	3.680		Crippen Method
mcvol	205.060	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55408496&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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