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/ci990307l
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