1H-Phenanthro[9,10-d]imidazole

Other names:	1,3-Diaza-1H-cyclopenta[1]phenanthrene
	9,10-Phenanthroimidazole
	Phenanthro(9,10)imidazole
Inchi:	InChI=1S/C15H10N2/c1-3-7-12-10(5-1)11-6-2-4-8-13(11)15-14(12)16-9-17-15/h1-9H,(H,
InchiKey:	WRQHNSKKYGHTLO-UHFFFAOYSA-N
Formula:	C15H10N2
SMILES:	c1ccc2c(c1)c1ccccc1c1[nH]cnc21
Mol. weight [g/mol]:	218.25
CAS:	236-02-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	3.387		Crippen Method
mcvol	164.330	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=C236022&Units=SI

Legend

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

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