

Benzo(a)phenazine

Inchi:	InChI=1S/C16H10N2/c1-2-6-12-11(5-1)9-10-15-16(12)18-14-8-4-3-7-13(14)17-15/h1-10H
InchiKey:	SEXRCKWGFSSXUOO-UHFFFAOYSA-N
Formula:	C16H10N2
SMILES:	c1ccc2c(c1)ccc1nc3ccccc3nc12
Mol. weight [g/mol]:	230.26
CAS:	225-61-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	3.936		Crippen Method
mcvol	174.120	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C225616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/89-583-7/Benzo-a-phenazine.pdf>

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