

Benzo[a]phenazine, 12-oxide

Inchi:	InChI=1S/C16H10N2O/c19-18-15-8-4-3-7-13(15)17-14-10-9-11-5-1-2-6-12(11)16(14)18/
InchiKey:	QOEUHFSHKLIUGS-UHFFFAOYSA-N
Formula:	C16H10N2O
SMILES:	[O-][n+]1c2ccccc2nc2ccc3ccccc3c21
Mol. weight [g/mol]:	246.26
CAS:	18636-87-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.18		Crippen Method
logp	3.175		Crippen Method
mcvol	179.990	ml/mol	McGowan Method

Sources

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=C18636878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/57-098-1/Benzo-a-phenazine-12-oxide.pdf>

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