

6,11-Dinitrobenzo[b]phenazine

Inchi:	InChI=1S/C16H8N4O4/c21-19(22)15-9-5-1-2-6-10(9)16(20(23)24)14-13(15)17-11-7-3-4-
InchiKey:	SPOWJHACBCKQGK-UHFFFAOYSA-N
Formula:	C16H8N4O4
SMILES:	O=[N+]([O-])c1c2ccccc2c([N+](=O)[O-])c2nc3ccccc3nc12
Mol. weight [g/mol]:	320.26
CAS:	97620-84-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.72		Crippen Method
logp	3.753		Crippen Method
mcvol	208.960	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=C97620843&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

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