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)17-11-7-3-4-8

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/ci990307l

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