

Phosphonic diamide, n,n'-bis (p-dimethylaniline)

Inchi: InChI=1S/C16H23N4OP/c1-19(2)15-9-5-13(6-10-15)17-22(21)18-14-7-11-16(12-8-14)20
InchiKey: XTWUDTRGWHGKLC-UHFFFAOYSA-N
Formula: C16H23N4OP
SMILES: CN(C)c1ccc(N=[PH](O)Nc2ccc(N(C)C)cc2)cc1
Mol. weight [g/mol]: 318.35
CAS: 116401-82-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.06		Crippen Method
logp	3.782		Crippen Method
mcvol	255.030	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=C116401822&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/74-120-6/Phosphonic-diamide-n-n-bis-p-dimethylaniline.pdf>

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