

Pyridine, 2,6-diamino-4-[(diphenylmethyl)amino]-3-nitro-

Inchi: InChI=1S/C18H17N5O2/c19-17-16(23(24)25)15(21-18(20)22-17)11-14(12-7-3-1-4-8-12)
InchiKey: YJLCLWFREUQTKL-UHFFFAOYSA-N
Formula: C18H17N5O2
SMILES: Nc1nc(N)c([N+](=O)[O-])c(CC(c2ccccc2)c2ccccc2)n1
Mol. weight [g/mol]: 335.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	2.924		Crippen Method
mcvol	250.540	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008447&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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