Pyridine, 1,1'-(1,2-phenylenedicarbonyl)bis[1,2,3,4-tetrahyd

Other names: Pyridine, 1,1'-(1,2-phenylenedicarbonyl)bis*1,2,3,4-tetrahydro-
Inchi: InChI=1S/C18H20N2O2/c21-17(19-11-5-1-6-12-19)15-9-3-4-10-16(15)18(22)20-13-7-2-8
InchiKey: PNANBGADSBTPED-UHFFFAOYSA-N
Formula: C18H20N2O2
SMILES: O=C(c1ccccc1C(=O)N1C=CCCC1)N1C=CCCC1
Mol. weight [g/mol]: 296.36
CAS: 52881-76-2

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
log10ws	-4.76		Crippen Method
logp	3.186		Crippen Method
mcvol	233.500	ml/mol	McGowan Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52881762&Units=SI

Legend

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