Pyridine, 1,1'-[1,2-phenylenebis(1-oxo-2,1-ethanediyl)]bis[1

Other names: Pyridine, 1,1'-[1,2-phenylenebis(1-oxo-2,1-ethanediyl)]bis*1,2,3,4-tetrahydro-
Inchi: InChI=1S/C20H24N2O2/c23-19(21-11-5-1-6-12-21)15-17-9-3-4-10-18(17)16-20(24)22-13
InchiKey: CQDVIEOVRSNWNY-UHFFFAOYSA-N
Formula: C20H24N2O2
SMILES: O=C(Cc1ccccc1CC(=O)N1C=CCCC1)N1C=CCCC1
Mol. weight [g/mol]: 324.42
CAS: 52881-80-8

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	NIST Webbook
log10ws	-4.44		Crippen Method
logp	3.044		Crippen Method
mcvol	261.680	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=C52881808&Units=SI

Legend

ie: Ionization energy
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/21-616-4/Pyridine-1-1-1-2-phenylenebis-1-oxo-2-1-ethanediyl-bis-1-2-3-4-tetrahydro.pd