

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

**Other names:** Pyridine, 1,1'-(1,4-phenylenedicarbonyl)bis\*1,2,3,4-tetrahydro-

**Inchi:** InChI=1S/C18H20N2O2/c21-17(19-11-3-1-4-12-19)15-7-9-16(10-8-15)18(22)20-13-5-2-6

**InchiKey:** KVGHIVIGUCJBQI-UHFFFAOYSA-N

**Formula:** C18H20N2O2

**SMILES:** O=C(c1ccc(C(=O)N2C=CCCC2)cc1)N1C=CCCC1

**Mol. weight [g/mol]:** 296.36

**CAS:** 52881-77-3

## 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

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C52881773&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**ie:** Ionization energy

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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