# Thenyldiamine

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|---|---|
| **Other names:** | 1,2-Ethanediamine, N,N-dimethyl-N'-2-pyridinyl-N'-(3-thienylmethyl)- |
| | Pyridine, 2-[[2-(dimethylamino)ethyl]-3-thenylamino]- |
| | Dethlandiamine |
| | Dethylandiamine |
| | Tenfidil |
| | Thefanil |
| | Thenfadil |
| | Thenyldiamine (pharmaceutical) |
| | WIN 2848 |
| | 2-[(2-Dimethylaminoethyl)-3-thenylamino]pyridine |
| | N-(2-Dimethylaminoethyl)-N-2-pyridyl-3-thenylamine |
| | N-(«alpha»-Pyridyl)-N-(«beta»-thenyl)-N',N'-dimethylethylenediamine |
| | NCI-C60640 |
| **Inchi:** | InChI=1S/C14H19N3S/c1-16(2)8-9-17(11-13-6-10-18-12-13)14-5-3-4-7-15-14/h3-7,10,12 |
| **InchiKey:** | RCGYDFVCAAKKNG-UHFFFAOYSA-N |
| **Formula:** | C14H19N3S |
| **SMILES:** | CN(C)CCN(Cc1ccsc1)c1ccccn1 |
| **Mol. weight [g/mol]:** | 261.39 |
| **CAS:** | 91-79-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.84 | | Crippen Method |
| logp | 2.711 | | Crippen Method |
| mcvol | 211.190 | ml/mol | McGowan Method |
| rinpol | 2005.00 | | NIST Webbook |
| rinpol | 1999.00 | | NIST Webbook |
| rinpol | 1963.00 | | NIST Webbook |
| rinpol | 2008.00 | | NIST Webbook |
| rinpol | 1992.00 | | NIST Webbook |
| rinpol | 1963.00 | | NIST Webbook |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C91792&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |