

1,2-Ethanediamine, N,N-dimethyl-N'-phenyl-N'-(2-thienylmethyl)-

Other names:	Ethylenediamine, N,N-dimethyl-N'-phenyl-N'-2-thenyl- Diatrin Diatrin base N,N-Dimethyl-N'-phenyl-N'-2-thenylethylenediamine Enstamine Methaphenilene R.P. 2740 W 50 Base N,N-Dimethyl-N'-(«alpha»-thenyl)-N'-phenethylenediamine RP-2740
Inchi:	InChI=1S/C15H20N2S/c1-16(2)10-11-17(13-15-9-6-12-18-15)14-7-4-3-5-8-14/h3-9,12H,1
InchiKey:	LDYJXVUOVPVZKA-UHFFFAOYSA-N
Formula:	C15H20N2S
SMILES:	CN(C)CCN(Cc1cccs1)c1cccc1
Mol. weight [g/mol]:	260.40
CAS:	493-78-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	3.316		Crippen Method
mcvol	215.300	ml/mol	McGowan Method
rinpola	1966.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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