METHAPHENILENE

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)c1ccccc1
Mol. weight [g/mol]:	260.41

Physical Properties

Property code	Value	Unit	Source
hvap	83.29	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	3.316		Crippen Method
mcvol	215.300	ml/mol	McGowan Method
rinpol	1966.00		NIST Webbook
tb	622.59	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493787&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature