Benzenamine, 4-(6-methyl-2-benzothiazolyl)-

Other names:	2-(4-Aminophenyl)-6-methylbenzothiazole
	2-(4-aminophenyl)-6-methyl-benzothiazole
	2-(p-Aminophenyl)-6-methylbenzothiazole
	4-(6-Methyl-2-benzethiazolyl)-benzeneamine
	4-(6-Methyl-2-benzothiazolyl)aniline
	4-(6-Methyl-2-benzothiazolyl)benzenamine
	4-(6-methylbenzothiazol-2-yl)aniline
	Benzothiazole, 2-(p-aminophenyl)-6-methyl-
	DHPT
	Dehydrothio-p-toluidine
	NSC 15370
	p-(6-Methylbenzothiazol-2-yl)aniline
Inchi:	InChI=1S/C14H12N2S/c1-9-2-7-12-13(8-9)17-14(16-12)10-3-5-11(15)6-4-10/h2-8H,15H2
InchiKey:	XRTJYEIMLZALBD-UHFFFAOYSA-N
Formula:	C14H12N2S
SMILES:	Cc1ccc2nc(-c3ccc(N)cc3)sc2c1
Mol. weight [g/mol]:	240.32
CAS:	92-36-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Aqueous Solubility Prediction Method
logp	3.854		Crippen Method
mcvol	181.750	ml/mol	McGowan Method
tb	707.20	K	NIST Webbook
tb	707.00	K	NIST Webbook
tf	467.95	K	Aqueous Solubility Prediction Method
tf	468.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92364&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point