

1,3,5-Triazine-2,4-diamine, N-cyclopropyl-N'-(1,1-dimethylethyl)-6-(methylthio)

Other names:	N-tert-Butyl-N'-cyclopropyl-6-methylsulfanyl-1,3,5-triazine-2,4-diamine N'-tert-butyl-N-cyclopropyl-6-(methylthio)-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C11H19N5S/c1-11(2,3)16-9-13-8(12-7-5-6-7)14-10(15-9)17-4/h7H,5-6H2,1-4H
InchiKey:	HDHLIWCXDDZUFH-UHFFFAOYSA-N
Formula:	C11H19N5S
SMILES:	CSc1nc(NC2CC2)nc(NC(C)(C)C)n1
Mol. weight [g/mol]:	253.37
CAS:	28159-98-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.378		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
rinpol	2095.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28159980&Units=SI

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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