Methoprotryne

Other names:	1,3,5-Triazine-2,4-diamine, N-(3-methoxypropyl)-N'-(1-methylethyl)-6-(methylthio)-
	2-Isopropylamino-4-(3-methoxypropylamino)-6-methylthio-1,3,5-triazine
	2-Isopropylamino-4-(3-methoxypropylamino)-6-methylthio-s-triazine
	2-Methylthio-4-isopropylamino-6-(3-methoxypropylamino)-s-triazine
	4-Isopropylamino-6-(3'-methoxypropylamino)-2-methythio-1,3,5-triazine
	G 36393
	Gesaran
	Gesaran 25
	Methoproptryne
	Methoproteryne
	Methoprotryn
	Methotryne
	Metoprotryn
	Metoprotryne
	s-Triazine, 2-(isopropylamino)-4-[(3-methoxypropyl)amino]-6-(methylthio)-
Inchi:	InChI=1S/C11H21N5OS/c1-8(2)13-10-14-9(12-6-5-7-17-3)15-11(16-10)18-4/h8H,5-7H2,1
InchiKey:	DDUIUBPJPOKOMV-UHFFFAOYSA-N
Formula:	C11H21N5OS
SMILES:	COCCCNc1nc(NC(C)C)nc(SC)n1
Mol. weight [g/mol]:	271.38
CAS:	841-06-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.93		Aqueous Solubility Prediction Method
log10ws	-2.93		Estimated Solubility Method
logp	1.862		Crippen Method
mcvol	214.210	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2150.00		NIST Webbook
ripol	3202.00		NIST Webbook
ripol	3202.00		NIST Webbook
ripol	3202.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C841065&Units=SI
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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

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