Aziprotryne

Other names:	1,3,5-Triazin-2-amine, 4-azido-N-(1-methylethyl)-6-(methylthio)- s-Triazine, 2-azido-4-(isopropylamino)-6-(methylthio)- Azeprotyrne 2-Azido-4-isopropylamino-6-methylthio-s-triazine 2-Azido-4-isopropylamino-6-methylthio-1,3,5-triazine 4-Azido-N-(1-methylethyl)-6-(methylthio)-1,3,5-triazin-2-amine Aziprotryn Azirpotryne Brasoran Brassoron C 7019 CIBA C 7019 Isopropylamino-4-azido-6-methylthio-1,3,5-triazin Mesoranil Mezaronil Mezuron
Inchi:	InChI=1S/C7H11N7S/c1-4(2)9-5-10-6(13-14-8)12-7(11-5)15-3/h4H,1-3H3,(H,9,10,11,12)
InchiKey:	AFIIBUOYKYSPKB-UHFFFAOYSA-N
Formula:	C7H11N7S
SMILES:	CSc1nc(N=[N+]=[N-])nc(NC(C)C)n1
Mol. weight [g/mol]:	225.27
CAS:	4658-28-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.13		Crippen Method
logp	2.356		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
rinpol	1766.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1766.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4658280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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