

2-Pyrimidinesulfonic acid, 4,6-diaminothio-, s-trichloromethyl ester

Inchi:	InChI=1S/C5H5Cl3N4O2S2/c6-5(7,8)15-16(13,14)4-11-2(9)1-3(10)12-4/h1H,(H4,9,10,11)
InchiKey:	ZTCNDLCKKPGTPZ-UHFFFAOYSA-N
Formula:	C5H5Cl3N4O2S2
SMILES:	<chem>Nc1cc(N)nc(S(=O)(=O)SC(Cl)(Cl)Cl)n1</chem>
Mol. weight [g/mol]:	323.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	1.391		Crippen Method
mcvol	178.630	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6008406&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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