Cyazofamid

Other names: 1H-Imidazole-1-sulfonamide, 4-chloro-2-cyano-N,N-dimethyl-5-(4-methylphenyl)-
4-chloro-2-cyano-N,N-dimethyl-5-(4-methylphenyl)-1H-imidazole-1-sulfonamide
Inchi: InChI=1S/C13H13ClN4O2S/c1-9-4-6-10(7-5-9)12-13(14)16-11(8-15)18(12)21(19,20)17(2
InchiKey: YXKMMRDKEKCERS-UHFFFAOYSA-N
Formula: C13H13ClN4O2S
SMILES: Cc1ccc(-c2c(Cl)nc(C#N)n2S(=O)(=O)N(C)C)cc1
Mol. weight [g/mol]: 324.79
CAS: 120116-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.61		Crippen Method
logp	2.038		Crippen Method
mcvol	222.460	ml/mol	McGowan Method
rinpol	2388.00		NIST Webbook
rinpol	2388.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120116883&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