

Pyrimidine, 2,5-bis(trifluoroacetamido)-4,6-bis(methylthio)-

Inchi:	InChI=1S/C10H8F6N4O2S2/c1-23-4-3(17-6(21)9(11,12)13)5(24-2)19-8(18-4)20-7(22)10
InchiKey:	SGHUHUDAJDQDEL-UHFFFAOYSA-N
Formula:	C10H8F6N4O2S2
SMILES:	CSc1nc(N=C(O)C(F)(F)F)nc(SC)c1N=C(O)C(F)(F)F
Mol. weight [g/mol]:	394.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	4.221		Crippen Method
mcvol	214.380	ml/mol	McGowan Method

Sources

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=B6008431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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