N-Isopropyl-N'-methyl-N,N'-bis(trifluoroacetyl)-6-m

Other names: 1,3,5-Triazine-2,4-diamine, N-methyl-N'-(1-methylethyl)-N,N'-bis-trifluoroacetyl-6-(methylthio)-
Inchi: InChI=1S/C12H13F6N5O2S/c1-5(2)23(7(25)12(16,17)18)9-19-8(20-10(21-9)26-4)22(3)6
InchiKey: LSHSXPWJOJLWCD-UHFFFAOYSA-N
Formula: C12H13F6N5O2S
SMILES: CSc1nc(N(C)C(=O)C(F)(F)F)nc(N(C(=O)C(F)(F)F)C(C)C)n1
Mol. weight [g/mol]: 405.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.422		Crippen Method
mcvol	236.190	ml/mol	McGowan Method
rinpol	1727.00		NIST Webbook
rinpol	1727.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373448&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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