N2-Cyclopropyl-1,3,5-triazine-2,4,6-triamine N2,N4,N6-tris(trifluoroacetate)

Other names: 1,3,5-Triazine-2,4,6-triamine, N2-cyclopropyl-N2,N4,N6-tris-trifluoroacetyl-
2,4,6-Tris-trifluoroacetylamino-6-(cyclopropylamino)-s-triazine
2-Cyclopropylamino-2,4,6-tris-trifluoroacetylamino-s-triazine

Inchi: InChI=1S/C12H7F9N6O3/c13-10(14,15)4(28)22-7-24-8(23-5(29)11(16,17)18)26-9(25-7)2

InchiKey: GBRJOJLXTAZOIS-UHFFFAOYSA-N

Formula: C12H7F9N6O3

SMILES: O=C(Nc1nc(NC(=O)C(F)(F)F)nc(N(C(=O)C(F)(F)F)C2CC2)n1)C(F)(F)F

Mol. weight [g/mol]: 454.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	1.931		Crippen Method
mcvol	225.840	ml/mol	McGowan Method
rinpol	1673.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U378207&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

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