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

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=U378207&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

Latest version available from:

https://www.chemeo.com/cid/47-270-0/N2-Cyclopropyl-1-3-5-triazine-2-4-6-triamine-N2-N4-N6-tris-trifluoroacetate.pd

Generated by Cheméo on 2024-10-12 06:06:34.88668517 +0000 UTC m=+3294057.523654418.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.