N-tert-Butyl-N,N'-bis(trifluoroacetyl)-6-methoxy-1,

Other names: 2-Trifluoroacetylamino-4-tert-butyl-4-trifluoroacetylamino-6-methoxy-1,3,5-triazine
6-Methoxy-N-(2-methyl-2-propanyl)-N,N'-bis(trifluoroacetyl)-1,3,5-triazine-2,4-diamine
Inchi: InChI=1S/C12H13F6N5O3/c1-10(2,3)23(6(25)12(16,17)18)8-20-7(21-9(22-8)26-4)19-5(2
InchiKey: CODZVNZYBUJIRS-UHFFFAOYSA-N
Formula: C12H13F6N5O3
SMILES: COc1nc(NC(=O)C(F)(F)F)nc(N(C(=O)C(F)(F)F)C(C)(C)C)n1
Mol. weight [g/mol]: 389.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	2.075		Crippen Method
mcvol	225.710	ml/mol	McGowan Method
rinpol	1571.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373304&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