N-tert-Butyl-N,N'-bis(trifluoroacetyl)-6-methoxy-1,3,5-triazine-2,4-diamine

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.

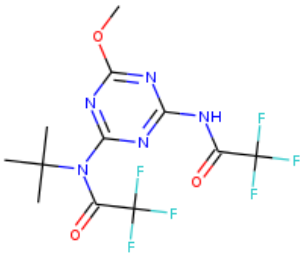
InChI: InChI=1S/C12H13F6N5O3/c1-10(2,3)23(6(25)12(16,17)18)8-20-7(21-9(22-8)26-4)19-5(24)11(13,14)15/h1-4H3,(H,19,20,21,22,24)

InChI Key: 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

Molecular Weight: 389.25



Physical Properties

Property	Value	Unit	Source
*log*P$_{oct/wat}$	2.07		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/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(24)11(13,14)15/h1-4H3,(H,19,20,21,22,24)

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .