

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.

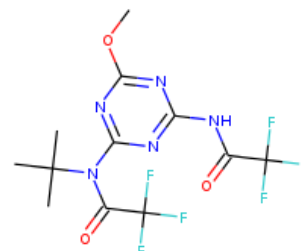
InChI: InChI=1S/C12H13F6N5O3/c1-10(2,3)23(6(25)12(16,17)18)8-20-7(21-9(22-8)26-4)19-5(24)11(13,14)15/h1-4H3,(H,19,20,21,22,24)

InChI Key: CODZVNZYBUJIRS-UHFFFAOYSA-N

Formula: C12H13F6N5O3

SMILES: COc1nc(NC(=O)C(F)(F)F)nc(NC(=O)C(F)(F)F)C(C)(C)C)n1

Molecular Weight: 389.25



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	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,\(H,19,20,21,22,24\)](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/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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