

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

|                             |                                                                                                                                                                               |
|-----------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Other names:</b>         | 2-Trifluoroacetylamino-4-tert-butyl-4-trifluoroacetylamino-6-methoxy-1,3,5-triazine<br>6-Methoxy-N-(2-methyl-2-propanyl)-N,N'-bis(trifluoroacetyl)-1,3,5-triazine-2,4-diamine |
| <b>Inchi:</b>               | 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                                                                                          |
| <b>InchiKey:</b>            | CODZVNZYBUJIRS-UHFFFAOYSA-N                                                                                                                                                   |
| <b>Formula:</b>             | C12H13F6N5O3                                                                                                                                                                  |
| <b>SMILES:</b>              | COc1nc(NC(=O)C(F)(F)F)nc(NC(=O)C(F)(F)F)C(C)(C)Cn1                                                                                                                            |
| <b>Mol. weight [g/mol]:</b> | 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

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373304&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinpol:</b>  | Non-polar retention indices         |

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