

4-(tert-Butylamino)-6-ethyl-6-trifluoroacetylaminotriazin-2-one

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| Other names: | 1,3,5-Triazin-2(1H)-one, 4-[[1,1-dimethylethylamino]-6-(ethylamino)-6-(trifluoroacetyl)amino]triazin-2(1H)-one |
| Inchi: | InChI=1S/C11H16F3N5O2/c1-5-19(6(20)11(12,13)14)8-15-7(16-9(21)17-8)18-10(2,3)4/h1 |
| InchiKey: | HNIOZFAQZIDXNR-UHFFFAOYSA-N |
| Formula: | C11H16F3N5O2 |
| SMILES: | CCN(C(=O)C(F)(F)F)c1nc(=O)nc(NC(C)(C)C)[nH]1 |
| Mol. weight [g/mol]: | 307.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.20 | | Crippen Method |
| logp | 0.809 | | Crippen Method |
| mcvol | 204.740 | ml/mol | McGowan Method |
| rinqol | 1116.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373153&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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

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