

**N-(2,2,3,3,4,4,4-Heptafluorobutanoyl)-N-(4-methox**

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Other names:</b>         | Bis(2,2,3,3,4,4,4-heptafluoro)-N-(4-methoxy-1,3-benzothiazol-2-yl)butyrylamide   |
| <b>Inchi:</b>               | InChI=1S/C16H6F14N2O3S/c1-35-5-3-2-4-6-7(5)31-10(36-6)32(8(33)11(17,18)13(21,22, |
| <b>InchiKey:</b>            | MTGBWUFHQMQQKP-UHFFFAOYSA-N                                                      |
| <b>Formula:</b>             | C16H6F14N2O3S                                                                    |
| <b>SMILES:</b>              | COc1cccc2sc(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F)nc12       |
| <b>Mol. weight [g/mol]:</b> | 572.27                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.47   |        | Crippen Method |
| logp          | 5.830   |        | Crippen Method |
| mcvol         | 267.480 | ml/mol | McGowan Method |
| rinpol        | 1958.00 |        | NIST Webbook   |
| rinpol        | 1958.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373334&Units=SI>

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

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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