# N-(1,2-Dimethylpropyl)-N,N-bis(heptafluorobutyry

**Inchi:** InChI=1S/C19H19F14N5O2S/c1-6-37(9(39)14(20,21)16(24,25)18(28,29)30)11-34-12(36-
**InchiKey:** HEFWKULPLPXMMF-UHFFFAOYSA-N
**Formula:** C19H19F14N5O2S
**SMILES:** CCN(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1nc(SC)nc(N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C(
**Mol. weight [g/mol]:** 647.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.93 | | Crippen Method |
| logp | 5.990 | | Crippen Method |
| mcvol | 348.980 | ml/mol | McGowan Method |
| rinpol | 1787.00 | | NIST Webbook |

## Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U373414&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## Legend

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