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

Other names: Bis(2,2,3,3,4,4,4-heptafluoro)-N-(4-methoxy-1,3-benzothiazol-2-yl)butyrylamide
Inchi: 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)
InchiKey: MTGBWUFHQMQQKP-UHFFFAOYSA-N
Formula: C16H6F14N2O3S
SMILES: 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
Mol. weight [g/mol]: 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

Legend

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