

N-(1,2-Dimethylpropyl)-N,N-bis(heptafluorobutyryl)-N-ethyl-6-methylsulfanyl-1,3-dioxane-2-sulfonamide

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)S(=O)(=O)C1CCSC1
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

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