N-(1,2-Dimethylpropyl)-N,N'-bis(trifluoroacetyl)-N'

Inchi: InChI=1S/C15H19F6N5O2S/c1-6-25(9(27)14(16,17)18)11-22-12(24-13(23-11)29-5)26(8(
InchiKey: DCZCCKMNQJGGJB-UHFFFAOYSA-N
Formula: C15H19F6N5O2S
SMILES: CCN(C(=O)C(F)(F)F)c1nc(SC)nc(N(C(=O)C(F)(F)F)C(C)C(C)C)n1
Mol. weight [g/mol]: 447.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.449		Crippen Method
mcvol	278.460	ml/mol	McGowan Method
rinpol	1855.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U373416&Units=SI

Legend

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