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

Inchi:	InChI=1S/C17H19F10N5O2S/c1-6-31(9(33)14(18,19)16(22,23)24)11-28-12(30-13(29-11
InchiKey:	JFCQZIQCBBJVOQ-UHFFFAOYSA-N
Formula:	C17H19F10N5O2S
SMILES:	CCN(C(=O)C(F)(F)C(F)(F)F)c1nc(SC)nc(N(C(=O)C(F)(F)C(F)(F)F)C(C)C(C)C)n1
Mol. weight [g/mol]:	547.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	4.719		Crippen Method
mcvol	313.720	ml/mol	McGowan Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373415&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

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