2-Acetylthiazole, PFBO # 1

Inchi: InChI=1S/C12H7F5N2OS/c1-5(12-18-2-3-21-12)19-20-4-6-7(13)9(15)11(17)10(16)8(6)14
InchiKey: HSSKYLXRINHHQN-UHFFFAOYSA-N
Formula: C12H7F5N2OS
SMILES: CC(=NOCc1c(F)c(F)c(F)c(F)c1F)c1nccs1
Mol. weight [g/mol]: 322.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	3.779		Crippen Method
mcvol	183.450	ml/mol	McGowan Method
rinpol	1711.00		NIST Webbook
rinpol	1711.00		NIST Webbook
ripol	2362.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R574631&Units=SI
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

Legend

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

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