Thiophen-2-carboxaldehyde, PFBO # 1

Inchi: InChI=1S/C12H6F5NOS/c13-8-7(9(14)11(16)12(17)10(8)15)5-19-18-4-6-2-1-3-20-6/h1-4
InchiKey: METWJGDJOIBXOU-UHFFFAOYSA-N
Formula: C12H6F5NOS
SMILES: Fc1c(F)c(F)c(CON=Cc2cccs2)c(F)c1F
Mol. weight [g/mol]: 307.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.994		Crippen Method
mcvol	173.470	ml/mol	McGowan Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2375.00		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=R575921&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
ripol: Polar retention indices