

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

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<https://www.chemeo.com/cid/71-153-3/Thiophen-2-carboxaldehyde-PFBO-1.pdf>

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