

Thiophene-2-thiol, S-trifluoroacetyl-

Inchi: InChI=1S/C6H3F3OS2/c7-6(8,9)5(10)12-4-2-1-3-11-4/h1-3H
InchiKey: GFGCIGKAZFLVBA-UHFFFAOYSA-N
Formula: C6H3F3OS2
SMILES: O=C(Sc1cccs1)C(F)(F)F
Mol. weight [g/mol]: 212.21

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.83 | | Crippen Method |
| logp | 2.929 | | Crippen Method |
| mcvol | 115.520 | ml/mol | McGowan Method |
| rinpol | 1027.00 | | NIST Webbook |
| rinpol | 1027.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375544&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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<https://www.chemeo.com/cid/118-481-7/Thiophene-2-thiol-S-trifluoroacetyl.pdf>

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