

2-Thiopheneacetic acid, 3,4-dichlorophenyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H8Cl2O2S/c13-10-4-3-8(6-11(10)14)16-12(15)7-9-2-1-5-17-9/h1-6H,7H2 |
| InchiKey: | BTHYDFCWZORZBJ-UHFFFAOYSA-N |
| Formula: | C12H8Cl2O2S |
| SMILES: | O=C(Cc1cccs1)Oc1ccc(Cl)c(Cl)c1 |
| Mol. weight [g/mol]: | 287.16 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.53 | | Crippen Method |
| logp | 4.203 | | Crippen Method |
| mcvol | 184.990 | ml/mol | McGowan Method |
| rinpol | 2077.00 | | NIST Webbook |
| rinpol | 2077.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308058&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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