

2-Thiopheneacetic acid, oct-3-en-2-yl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C14H20O2S/c1-3-4-5-6-8-12(2)16-14(15)11-13-9-7-10-17-13/h6-10,12H,3-5,1 |
| InchiKey: | YDNAYZGNNTUALT-SOFGYWHQSA-N |
| Formula: | C14H20O2S |
| SMILES: | CCCCC=CC(C)OC(=O)Cc1cccs1 |
| Mol. weight [g/mol]: | 252.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.21 | | Crippen Method |
| logp | 3.969 | | Crippen Method |
| mcvol | 208.150 | ml/mol | McGowan Method |
| rinpole | 1717.00 | | NIST Webbook |
| rinpole | 1717.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U299386&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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

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