

Thiophene, 3-(2-methylpropyl)thio

Inchi: InChI=1S/C8H12S2/c1-7(2)5-10-8-3-4-9-6-8/h3-4,6-7H,5H2,1-2H3
InchiKey: MYUHABQFQLJLKR-UHFFFAOYSA-N
Formula: C8H12S2
SMILES: CC(C)CSc1ccsc1
Mol. weight [g/mol]: 172.31

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.99 | | Crippen Method |
| logp | 3.496 | | Crippen Method |
| mcvol | 136.820 | ml/mol | McGowan Method |
| rinpol | 1272.00 | | NIST Webbook |
| rinpol | 1277.00 | | NIST Webbook |
| rinpol | 1282.00 | | NIST Webbook |
| rinpol | 1262.00 | | NIST Webbook |
| rinpol | 1260.00 | | NIST Webbook |
| rinpol | 1264.00 | | NIST Webbook |
| rinpol | 1262.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R57779&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/48-304-1/Thiophene-3-2-methylpropyl-thio.pdf>

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