

# 4-(2,2'-Bithiophen-5-yl)but-3-yn-1-ol

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C12H10OS2/c13-8-2-1-4-10-6-7-12(15-10)11-5-3-9-14-11/h3,5-7,9,13H,2,8H2 |
| InchiKey:            | ASKPCVROMAYWEF-UHFFFAOYSA-N                                                      |
| Formula:             | C12H10OS2                                                                        |
| SMILES:              | OCCC#Cc1ccc(-c2cccs2)s1                                                          |
| Mol. weight [g/mol]: | 234.34                                                                           |
| CAS:                 | 1137-87-7                                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.39   |        | Crippen Method |
| logp          | 3.211   |        | Crippen Method |
| mcvol         | 170.990 | ml/mol | McGowan Method |
| rinpol        | 2222.00 |        | NIST Webbook   |
| rinpol        | 2215.10 |        | NIST Webbook   |
| rinpol        | 2215.10 |        | NIST Webbook   |
| rinpol        | 2222.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1137877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1137877&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## 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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