

# Sarcosine, N-(2-thienylcarbonyl)-, isohexyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C14H21NO3S/c1-11(2)6-4-8-18-13(16)10-15(3)14(17)12-7-5-9-19-12/h5,7,9,1 |
| InchiKey:            | AMMJBQUSLZXEPF-UHFFFAOYSA-N  |
| Formula:             | C14H21NO3S   |
| SMILES:              | CC(C)CCCOC(=O)CN(C)C(=O)c1cccs1  |
| Mol. weight [g/mol]: | 283.39   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.92   |        | Crippen Method |
| logp          | 2.800   |        | Crippen Method |
| mcvol         | 224.000 | ml/mol | McGowan Method |
| rinpola       | 2188.00 |        | NIST Webbook   |
| rinpola       | 2188.00 |        | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321466&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321466&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

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