

# (Phenylthio)acetic acid, tetradecyl ester

**Inchi:** InChI=1S/C22H36O2S/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-24-22(23)20-25-21-17-14-13-15  
**InchiKey:** CSISNRHHVYWFNT-UHFFFAOYSA-N  
**Formula:** C22H36O2S  
**SMILES:** CCCCCCCCCCCCCOC(=O)CSc1ccccc1  
**Mol. weight [g/mol]:** 364.58

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 45.97   | kJ/mol  | Joback Method  |
| hf            | -463.81 | kJ/mol  | Joback Method  |
| hfus          | 53.69   | kJ/mol  | Joback Method  |
| hvap          | 82.81   | kJ/mol  | Joback Method  |
| log10ws       | -7.36   |         | Crippen Method |
| logp          | 7.023   |         | Crippen Method |
| mcvol         | 320.870 | ml/mol  | McGowan Method |
| pc            | 1160.08 | kPa     | Joback Method  |
| rinpol        | 2712.00 |         | NIST Webbook   |
| tb            | 874.51  | K       | Joback Method  |
| tc            | 1079.49 | K       | Joback Method  |
| tf            | 470.68  | K       | Joback Method  |
| vc            | 1.238   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1011.35 | J/mol×K | 874.51          | Joback Method |
| cpg           | 1028.92 | J/mol×K | 908.67          | Joback Method |
| cpg           | 1045.24 | J/mol×K | 942.84          | Joback Method |
| cpg           | 1060.38 | J/mol×K | 977.00          | Joback Method |
| cpg           | 1074.36 | J/mol×K | 1011.16         | Joback Method |
| cpg           | 1087.23 | J/mol×K | 1045.33         | Joback Method |
| cpg           | 1099.04 | J/mol×K | 1079.49         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299851&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299851&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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