

# N-Benzyl O-propyl thiocarbamate

**Inchi:** InChI=1S/C11H15NOS/c1-2-8-13-11(14)12-9-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,  
**InchiKey:** KTOIPILWYSRXQY-UHFFFAOYSA-N  
**Formula:** C11H15NOS  
**SMILES:** CCCOC(S)=NCc1ccccc1  
**Mol. weight [g/mol]:** 209.31

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -55.15  | kJ/mol | Joback Method  |
| hvap          | 54.90   | kJ/mol | Joback Method  |
| log10ws       | -3.34   |        | Crippen Method |
| logp          | 2.899   |        | Crippen Method |
| mcvol         | 169.990 | ml/mol | McGowan Method |
| pc            | 2510.03 | kPa    | Joback Method  |
| rinpol        | 1784.00 |        | NIST Webbook   |
| rinpol        | 1784.00 |        | NIST Webbook   |
| ripol         | 2868.00 |        | NIST Webbook   |
| ripol         | 2868.00 |        | NIST Webbook   |
| tb            | 639.60  | K      | Joback Method  |
| tc            | 879.51  | K      | Joback Method  |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R440023&Units=SI>

## Legend

|                 |   |
|-----------------|---|
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hvac:</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>ripola:</b>  | Polar retention indices                         |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |

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