# Phenylthioacetamide, N,N-dihexyl-

**Inchi:** InChI=1S/C20H33NOS/c1-3-5-7-12-16-21(17-13-8-6-4-2)20(22)18-23-19-14-10-9-11-15-

**InchiKey:** YFLBMMZUHJDQBH-UHFFFAOYSA-N

**Formula:** C20H33NOS

**SMILES:** CCCCCCN(CCCCCC)C(=O)CSc1ccccc1

**Mol. weight [g/mol]:** 335.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 244.91 | kJ/mol | Joback Method |
| hf | -222.78 | kJ/mol | Joback Method |
| hfus | 50.35 | kJ/mol | Joback Method |
| hvap | 78.00 | kJ/mol | Joback Method |
| log10ws | -6.00 | | Crippen Method |
| logp | 5.768 | | Crippen Method |
| mcvol | 296.800 | ml/mol | McGowan Method |
| pc | 1342.74 | kPa | Joback Method |
| rinpol | 2538.00 | | NIST Webbook |
| tb | 818.77 | K | Joback Method |
| tc | 1021.73 | K | Joback Method |
| tf | 458.38 | K | Joback Method |
| vc | 1.125 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 903.77 | J/mol×K | 818.77 | Joback Method |
| cpg | 921.52 | J/mol×K | 852.60 | Joback Method |
| cpg | 938.13 | J/mol×K | 886.42 | Joback Method |
| cpg | 953.65 | J/mol×K | 920.25 | Joback Method |
| cpg | 968.14 | J/mol×K | 954.08 | Joback Method |
| cpg | 981.65 | J/mol×K | 987.90 | Joback Method |
| cpg | 994.25 | J/mol×K | 1021.73 | Joback Method |

# Sources

| | |
|---|---|
| **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=U308160&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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