

# N,n-diethyl-p-methoxy-phenoxy propylamine

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C14H23NO2/c1-4-15(5-2)11-6-12-17-14-9-7-13(16-3)8-10-14/h7-10H,4-6,11-1 |
| <b>InchiKey:</b>            | XGMGMACKPMSEOD-UHFFFAOYSA-N                                                      |
| <b>Formula:</b>             | C14H23NO2                                                                        |
| <b>SMILES:</b>              | CCN(CC)CCCOc1ccc(OC)cc1                                                          |
| <b>Mol. weight [g/mol]:</b> | 237.34                                                                           |
| <b>CAS:</b>                 | 58469-70-8                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 70.56   | kJ/mol  | Joback Method  |
| hf            | -304.14 | kJ/mol  | Joback Method  |
| hfus          | 31.06   | kJ/mol  | Joback Method  |
| hvap          | 56.56   | kJ/mol  | Joback Method  |
| log10ws       | -2.79   |         | Crippen Method |
| logp          | 2.806   |         | Crippen Method |
| mcvol         | 206.080 | ml/mol  | McGowan Method |
| pc            | 1920.30 | kPa     | Joback Method  |
| tb            | 608.66  | K       | Joback Method  |
| tc            | 798.62  | K       | Joback Method  |
| tf            | 363.41  | K       | Joback Method  |
| vc            | 0.765   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 536.34 | J/molxK | 608.66          | Joback Method |
| cpg           | 553.79 | J/molxK | 640.32          | Joback Method |
| cpg           | 570.36 | J/molxK | 671.98          | Joback Method |
| cpg           | 586.09 | J/molxK | 703.64          | Joback Method |
| cpg           | 600.98 | J/molxK | 735.30          | Joback Method |
| cpg           | 615.06 | J/molxK | 766.96          | Joback Method |
| cpg           | 628.34 | J/molxK | 798.62          | 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=C58469708&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C58469708&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>h vap:</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>m cvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <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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