

5-Phenoxymethyl-3-phenyl-2-oxazolidone

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|-----------------------------|--|
| Other names: | 3-Phenyl-5-phenoxyethyl-2-oxazolidinone |
| Inchi: | InChI=1S/C16H15NO3/c18-16-17(13-7-3-1-4-8-13)11-15(20-16)12-19-14-9-5-2-6-10-14/ |
| InchiKey: | TVCILYMEQCWTGP-UHFFFAOYSA-N |
| Formula: | C16H15NO3 |
| SMILES: | O=C1OC(COc2ccccc2)CN1c1ccccc1 |
| Mol. weight [g/mol]: | 269.30 |
| CAS: | 1226-26-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|---------|----------------|
| chs | -8022.40 ± 5.00 | kJ/mol | NIST Webbook |
| hfs | -417.60 ± 5.00 | kJ/mol | NIST Webbook |
| log10ws | -3.41 | | Crippen Method |
| logp | 3.091 | | Crippen Method |
| mcvol | 201.210 | ml/mol | McGowan Method |
| ss | 330.00 | J/mol×K | NIST Webbook |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|--------------|
| cps | 310.60 | J/mol×K | 298.15 | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1226262&Units=SI |

Legend

| | |
|-----------------|--|
| chs: | Standard solid enthalpy of combustion |
| cps: | Solid phase heat capacity |
| hfs: | Solid phase enthalpy of formation at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| ss: | Solid phase molar entropy at standard conditions |

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