

Benzoic acid, 2-phenoxy-

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| Other names: | Benzoic acid, o-phenoxy- o-Phenoxybenzoic acid 2-Phenoxybenzoic acid ortho-Phenoxybenzoic acid |
| Inchi: | InChI=1S/C13H10O3/c14-13(15)11-8-4-5-9-12(11)16-10-6-2-1-3-7-10/h1-9H,(H,14,15) |
| InchiKey: | PKRSYEPBQPFNRB-UHFFFAOYSA-N |
| Formula: | C13H10O3 |
| SMILES: | O=C(O)c1ccccc1Oc1ccccc1 |
| Mol. weight [g/mol]: | 214.22 |
| CAS: | 2243-42-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -96.97 | kJ/mol | Joback Method |
| hf | -247.09 | kJ/mol | Joback Method |
| hfus | 23.99 | kJ/mol | Joback Method |
| hvap | 75.58 | kJ/mol | Joback Method |
| log10ws | -3.17 | | Crippen Method |
| logp | 3.177 | | Crippen Method |
| mcvol | 159.820 | ml/mol | McGowan Method |
| pc | 3538.87 | kPa | Joback Method |
| tb | 723.65 | K | Joback Method |
| tc | 951.31 | K | Joback Method |
| tf | 434.61 | K | Joback Method |
| vc | 0.591 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 413.87 | J/molxK | 723.65 | Joback Method |
| cpg | 461.11 | J/molxK | 913.37 | Joback Method |
| cpg | 453.33 | J/molxK | 875.43 | Joback Method |
| cpg | 444.75 | J/molxK | 837.48 | Joback Method |
| cpg | 435.34 | J/molxK | 799.54 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 425.06 | J/molxK | 761.59 | Joback Method |
| cpg | 468.14 | J/molxK | 951.31 | Joback Method |
| dvisc | 0.0000378 | Paxs | 723.65 | Joback Method |
| dvisc | 0.0000541 | Paxs | 675.48 | Joback Method |
| dvisc | 0.0000819 | Paxs | 627.30 | Joback Method |
| dvisc | 0.0001326 | Paxs | 579.13 | Joback Method |
| dvisc | 0.0002344 | Paxs | 530.96 | Joback Method |
| dvisc | 0.0004645 | Paxs | 482.78 | Joback Method |
| dvisc | 0.0010708 | Paxs | 434.61 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| 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=C2243427&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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