

Phenol, o-(o-methoxyphenoxy)-

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|-----------------------------|--|
| Other names: | 2-(2-Methoxyphenoxy)phenol 2-Hydroxy-2'-methoxy diphenyl ether |
| Inchi: | InChI=1S/C13H12O3/c1-15-12-8-4-5-9-13(12)16-11-7-3-2-6-10(11)14/h2-9,14H,1H3 |
| InchiKey: | OHMCFTVLHBWELH-UHFFFAOYSA-N |
| Formula: | C13H12O3 |
| SMILES: | COc1ccccc1Oc1ccccc1O |
| Mol. weight [g/mol]: | 216.23 |
| CAS: | 21905-60-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -90.85 | kJ/mol | Joback Method |
| hf | -291.81 | kJ/mol | Joback Method |
| hfus | 25.28 | kJ/mol | Joback Method |
| hvap | 67.58 | kJ/mol | Joback Method |
| log10ws | -2.77 | | Crippen Method |
| logp | 3.193 | | Crippen Method |
| mvol | 164.120 | ml/mol | McGowan Method |
| pc | 3443.98 | kPa | Joback Method |
| tb | 680.64 | K | Joback Method |
| tc | 927.48 | K | Joback Method |
| tf | 457.81 | K | Joback Method |
| vc | 0.549 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 424.64 | J/molxK | 680.64 | Joback Method |
| cpg | 484.28 | J/molxK | 886.34 | Joback Method |
| cpg | 474.03 | J/molxK | 845.20 | Joback Method |
| cpg | 463.02 | J/molxK | 804.06 | Joback Method |
| cpg | 451.17 | J/molxK | 762.92 | Joback Method |
| cpg | 438.41 | J/molxK | 721.78 | Joback Method |
| cpg | 493.86 | J/molxK | 927.48 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000127 | Paxs | 680.64 | Joback Method |
| dvisc | 0.0000184 | Paxs | 643.50 | Joback Method |
| dvisc | 0.0000277 | Paxs | 606.36 | Joback Method |
| dvisc | 0.0000440 | Paxs | 569.23 | Joback Method |
| dvisc | 0.0000746 | Paxs | 532.09 | Joback Method |
| dvisc | 0.0001369 | Paxs | 494.95 | Joback Method |
| dvisc | 0.0002772 | Paxs | 457.81 | 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=C21905602&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

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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