

Benzene, 1-methoxy-3-phenoxy-

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|-----------------------------|---|
| Other names: | m-Methoxyphenyl phenyl ether m-Phenoxy methoxybenzene m-Phenoxyphenol monomethyl ether 1-Methoxy-3-phenoxybenzene 3-Methoxyphenoxybenzene Benzene, 1-methoxy-3-phenyloxy m-phenoxyanisole |
| Inchi: | InChI=1S/C13H12O2/c1-14-12-8-5-9-13(10-12)15-11-6-3-2-4-7-11/h2-10H,1H3 |
| InchiKey: | CBVXNDCIOLXDFD-UHFFFAOYSA-N |
| Formula: | C13H12O2 |
| SMILES: | COc1cccc(Oc2ccccc2)c1 |
| Mol. weight [g/mol]: | 200.23 |
| CAS: | 1655-68-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 63.77 | kJ/mol | Joback Method |
| hf | -114.50 | kJ/mol | Joback Method |
| hfus | 19.50 | kJ/mol | Joback Method |
| hvap | 54.57 | kJ/mol | Joback Method |
| log10ws | -3.23 | | Crippen Method |
| logp | 3.487 | | Crippen Method |
| mcvol | 158.250 | ml/mol | McGowan Method |
| pc | 2912.39 | kPa | Joback Method |
| tb | 600.02 | K | Joback Method |
| tc | 838.46 | K | Joback Method |
| tf | 346.09 | K | Joback Method |
| vc | 0.584 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 374.17 | J/mol×K | 600.02 | Joback Method |
| cpg | 442.69 | J/mol×K | 798.72 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 431.05 | J/molxK | 758.98 | Joback Method |
| cpg | 418.41 | J/molxK | 719.24 | Joback Method |
| cpg | 404.72 | J/molxK | 679.50 | Joback Method |
| cpg | 389.98 | J/molxK | 639.76 | Joback Method |
| cpg | 453.34 | J/molxK | 838.46 | Joback Method |
| dvisc | 0.0001253 | Paxs | 600.02 | Joback Method |
| dvisc | 0.0001572 | Paxs | 557.70 | Joback Method |
| dvisc | 0.0002047 | Paxs | 515.38 | Joback Method |
| dvisc | 0.0002795 | Paxs | 473.06 | Joback Method |
| dvisc | 0.0004057 | Paxs | 430.73 | Joback Method |
| dvisc | 0.0006388 | Paxs | 388.41 | Joback Method |
| dvisc | 0.0011238 | Paxs | 346.09 | 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=C1655681&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 |
| 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 |
| mccvol: | 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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