

1,6-Di-(4-bromophenoxy)hexane

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|-----------------------------|---|
| Other names: | benzene, 1,1'-[1,6-hexanediylbis(oxy)]bis-4-bromo- |
| Inchi: | InChI=1S/C18H20Br2O2/c19-15-5-9-17(10-6-15)21-13-3-1-2-4-14-22-18-11-7-16(20)8-12 |
| InchiKey: | RCTHJRFRURADHF-UHFFFAOYSA-N |
| Formula: | C18H20Br2O2 |
| SMILES: | BrC1ccc(OCCCCCOc2ccc(Br)cc2)cc1 |
| Mol. weight [g/mol]: | 428.16 |
| CAS: | 6943-11-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 124.88 | kJ/mol | Joback Method |
| hf | -176.51 | kJ/mol | Joback Method |
| hfus | 42.63 | kJ/mol | Joback Method |
| hvap | 79.23 | kJ/mol | Joback Method |
| log10ws | -7.36 | | Crippen Method |
| logp | 6.230 | | Crippen Method |
| mcvol | 263.700 | ml/mol | McGowan Method |
| pc | 2047.46 | kPa | Joback Method |
| tb | 851.72 | K | Joback Method |
| tc | 1088.92 | K | Joback Method |
| tf | 534.56 | K | Joback Method |
| vc | 0.988 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 713.00 | J/molxK | 851.72 | Joback Method |
| cpg | 727.06 | J/molxK | 891.25 | Joback Method |
| cpg | 739.97 | J/molxK | 930.79 | Joback Method |
| cpg | 751.79 | J/molxK | 970.32 | Joback Method |
| cpg | 762.57 | J/molxK | 1009.85 | Joback Method |
| cpg | 772.38 | J/molxK | 1049.38 | Joback Method |
| cpg | 781.27 | J/molxK | 1088.92 | Joback Method |
| dvisc | 0.0003542 | Paxs | 534.56 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002217 | Paxs | 587.42 | Joback Method |
| dvisc | 0.0001499 | Paxs | 640.28 | Joback Method |
| dvisc | 0.0001076 | Paxs | 693.14 | Joback Method |
| dvisc | 0.0000810 | Paxs | 746.00 | Joback Method |
| dvisc | 0.0000633 | Paxs | 798.86 | Joback Method |
| dvisc | 0.0000510 | Paxs | 851.72 | 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=C6943119&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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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