# Phthalic acid, 5-bromo-2-methoxybenzyl hexyl ester

**Inchi:** InChI=1S/C22H25BrO5/c1-3-4-5-8-13-27-21(24)18-9-6-7-10-19(18)22(25)28-15-16-14-1
**InchiKey:** YUYLWQZNHNXRAO-UHFFFAOYSA-N
**Formula:** C22H25BrO5
**SMILES:** CCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Br)ccc1OC
**Mol. weight [g/mol]:** 449.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -228.23 | kJ/mol | Joback Method |
| hf | -654.25 | kJ/mol | Joback Method |
| hfus | 51.70 | kJ/mol | Joback Method |
| hvap | 98.26 | kJ/mol | Joback Method |
| log10ws | -7.44 | | Crippen Method |
| logp | 5.552 | | Crippen Method |
| mcvol | 311.570 | ml/mol | McGowan Method |
| pc | 1515.21 | kPa | Joback Method |
| rinpol | 2997.00 | | NIST Webbook |
| rinpol | 2997.00 | | NIST Webbook |
| tb | 1012.22 | K | Joback Method |
| tc | 1247.22 | K | Joback Method |
| tf | 654.45 | K | Joback Method |
| vc | 1.179 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 954.54 | J/mol×K | 1012.22 | Joback Method |
| cpg | 965.65 | J/mol×K | 1051.39 | Joback Method |
| cpg | 975.26 | J/mol×K | 1090.55 | Joback Method |
| cpg | 983.41 | J/mol×K | 1129.72 | Joback Method |
| cpg | 990.11 | J/mol×K | 1168.89 | Joback Method |
| cpg | 995.41 | J/mol×K | 1208.06 | Joback Method |
| cpg | 999.32 | J/mol×K | 1247.22 | Joback Method |
| dvisc | 0.0001629 | Pa×s | 654.45 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001051 | Pa×s | 714.08 | Joback Method |
| dvisc | 0.0000725 | Pa×s | 773.71 | Joback Method |
| dvisc | 0.0000527 | Pa×s | 833.34 | Joback Method |
| dvisc | 0.0000400 | Pa×s | 892.96 | Joback Method |
| dvisc | 0.0000315 | Pa×s | 952.59 | Joback Method |
| dvisc | 0.0000254 | Pa×s | 1012.22 | Joback Method |

# Sources

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|---|---|
| **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=U382868&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 |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |