# Phthalic acid, 2-(3-bromophenyl)ethyl hexyl ester

**Inchi:** InChI=1S/C22H25BrO4/c1-2-3-4-7-14-26-21(24)19-11-5-6-12-20(19)22(25)27-15-13-17-9

**InchiKey:** JLTCLWBMSQWPQS-UHFFFAOYSA-N

**Formula:** C22H25BrO4

**SMILES:** CCCCCCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

**Mol. weight [g/mol]:** 433.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -113.60 | kJ/mol | Joback Method |
| hf | -510.56 | kJ/mol | Joback Method |
| hfus | 50.90 | kJ/mol | Joback Method |
| hvap | 95.19 | kJ/mol | Joback Method |
| log10ws | -7.25 | | Crippen Method |
| logp | 5.586 | | Crippen Method |
| mcvol | 305.700 | ml/mol | McGowan Method |
| pc | 1553.67 | kPa | Joback Method |
| rinpol | 2988.00 | | NIST Webbook |
| rinpol | 2988.00 | | NIST Webbook |
| tb | 984.82 | K | Joback Method |
| tc | 1217.88 | K | Joback Method |
| tf | 619.70 | K | Joback Method |
| vc | 1.161 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 930.34 | J/mol×K | 984.82 | Joback Method |
| cpg | 942.66 | J/mol×K | 1023.66 | Joback Method |
| cpg | 953.69 | J/mol×K | 1062.51 | Joback Method |
| cpg | 963.48 | J/mol×K | 1101.35 | Joback Method |
| cpg | 972.10 | J/mol×K | 1140.19 | Joback Method |
| cpg | 979.60 | J/mol×K | 1179.04 | Joback Method |
| cpg | 986.02 | J/mol×K | 1217.88 | Joback Method |
| dvisc | 0.0002520 | Pa×s | 619.70 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001550 | Pa×s | 680.55 | Joback Method |
| dvisc | 0.0001033 | Pa×s | 741.41 | Joback Method |
| dvisc | 0.0000732 | Pa×s | 802.26 | Joback Method |
| dvisc | 0.0000544 | Pa×s | 863.11 | Joback Method |
| dvisc | 0.0000421 | Pa×s | 923.97 | Joback Method |
| dvisc | 0.0000336 | Pa×s | 984.82 | 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=U378025&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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