# Diethylmalonic acid, 4-bromo-2-methoxyphenyl hexyl ester

**Inchi:** InChI=1S/C20H29BrO5/c1-5-8-9-10-13-25-18(22)20(6-2,7-3)19(23)26-16-12-11-15(21)14

**InchiKey:** SHDNEOLLXNVUPM-UHFFFAOYSA-N

**Formula:** C20H29BrO5

**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC

**Mol. weight [g/mol]:** 429.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -345.01 | kJ/mol | Joback Method |
| hf | -846.78 | kJ/mol | Joback Method |
| hfus | 45.45 | kJ/mol | Joback Method |
| hvap | 89.58 | kJ/mol | Joback Method |
| log10ws | -6.29 | | Crippen Method |
| logp | 5.293 | | Crippen Method |
| mcvol | 307.150 | ml/mol | McGowan Method |
| pc | 1398.55 | kPa | Joback Method |
| rinpol | 2543.00 | | NIST Webbook |
| tb | 931.57 | K | Joback Method |
| tc | 1149.49 | K | Joback Method |
| tf | 595.39 | K | Joback Method |
| vc | 1.165 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 945.57 | J/mol×K | 931.57 | Joback Method |
| cpg | 959.41 | J/mol×K | 967.89 | Joback Method |
| cpg | 972.02 | J/mol×K | 1004.21 | Joback Method |
| cpg | 983.42 | J/mol×K | 1040.53 | Joback Method |
| cpg | 993.66 | J/mol×K | 1076.85 | Joback Method |
| cpg | 1002.78 | J/mol×K | 1113.17 | Joback Method |
| cpg | 1010.81 | J/mol×K | 1149.49 | Joback Method |
| dvisc | 0.0002086 | Pa×s | 595.39 | Joback Method |
| dvisc | 0.0001257 | Pa×s | 651.42 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000820 | Pa×s | 707.45 | Joback Method |
| dvisc | 0.0000570 | Pa×s | 763.48 | Joback Method |
| dvisc | 0.0000416 | Pa×s | 819.51 | Joback Method |
| dvisc | 0.0000317 | Pa×s | 875.54 | Joback Method |
| dvisc | 0.0000249 | Pa×s | 931.57 | Joback Method |

# Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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=U370949&Units=SI

# 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