# Diethylmalonic acid, 4-bromophenyl octyl ester

**Inchi:** InChI=1S/C21H31BrO4/c1-4-7-8-9-10-11-16-25-19(23)21(5-2,6-3)20(24)26-18-14-12-17(

**InchiKey:** IDYDIWDKIOFCIL-UHFFFAOYSA-N

**Formula:** C21H31BrO4

**SMILES:** CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1

**Mol. weight [g/mol]:** 427.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -221.96 | kJ/mol | Joback Method |
| hf | -723.73 | kJ/mol | Joback Method |
| hfus | 47.24 | kJ/mol | Joback Method |
| hvap | 88.73 | kJ/mol | Joback Method |
| log10ws | -7.01 | | Crippen Method |
| logp | 6.065 | | Crippen Method |
| mcvol | 315.370 | ml/mol | McGowan Method |
| pc | 1333.93 | kPa | Joback Method |
| rinpol | 2576.00 | | NIST Webbook |
| rinpol | 2576.00 | | NIST Webbook |
| tb | 927.05 | K | Joback Method |
| tc | 1143.73 | K | Joback Method |
| tf | 571.91 | K | Joback Method |
| vc | 1.202 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 978.07 | J/mol×K | 927.05 | Joback Method |
| cpg | 992.85 | J/mol×K | 963.16 | Joback Method |
| cpg | 1006.49 | J/mol×K | 999.28 | Joback Method |
| cpg | 1019.04 | J/mol×K | 1035.39 | Joback Method |
| cpg | 1030.58 | J/mol×K | 1071.50 | Joback Method |
| cpg | 1041.16 | J/mol×K | 1107.62 | Joback Method |
| cpg | 1050.85 | J/mol×K | 1143.73 | Joback Method |
| dvisc | 0.0003024 | Pa×s | 571.91 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001694 | Pa×s | 631.10 | Joback Method |
| dvisc | 0.0001049 | Pa×s | 690.29 | Joback Method |
| dvisc | 0.0000700 | Pa×s | 749.48 | Joback Method |
| dvisc | 0.0000496 | Pa×s | 808.67 | Joback Method |
| dvisc | 0.0000368 | Pa×s | 867.86 | Joback Method |
| dvisc | 0.0000284 | Pa×s | 927.05 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U369827&Units=SI |
| **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 |

# 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 |