# Dimethylmalonic acid, 2-bromo-4-fluorophenyl pentyl ester

**Inchi:** InChI=1S/C16H20BrFO4/c1-4-5-6-9-21-14(19)16(2,3)15(20)22-13-8-7-11(18)10-12(13)1

**InchiKey:** PCVXHMAKAJWUOT-UHFFFAOYSA-N

**Formula:** C16H20BrFO4

**SMILES:** CCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)cc1Br

**Mol. weight [g/mol]:** 375.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -468.50 | kJ/mol | Joback Method |
| hf | -828.11 | kJ/mol | Joback Method |
| hfus | 36.98 | kJ/mol | Joback Method |
| hvap | 77.44 | kJ/mol | Joback Method |
| log10ws | -5.25 | | Crippen Method |
| logp | 4.253 | | Crippen Method |
| mcvol | 246.690 | ml/mol | McGowan Method |
| pc | 1861.11 | kPa | Joback Method |
| rinpol | 2009.00 | | NIST Webbook |
| rinpol | 2009.00 | | NIST Webbook |
| tb | 816.90 | K | Joback Method |
| tc | 1030.99 | K | Joback Method |
| tf | 528.67 | K | Joback Method |
| vc | 0.941 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 695.59 | J/mol×K | 816.90 | Joback Method |
| cpg | 708.71 | J/mol×K | 852.58 | Joback Method |
| cpg | 720.83 | J/mol×K | 888.26 | Joback Method |
| cpg | 732.01 | J/mol×K | 923.94 | Joback Method |
| cpg | 742.27 | J/mol×K | 959.63 | Joback Method |
| cpg | 751.65 | J/mol×K | 995.31 | Joback Method |
| cpg | 760.20 | J/mol×K | 1030.99 | 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=U361822&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 |
| **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 |