# Succinic acid, dec-2-yl 2-bromo-4-fluorophenyl ester

**Inchi:** InChI=1S/C20H28BrFO4/c1-3-4-5-6-7-8-9-15(2)25-19(23)12-13-20(24)26-18-11-10-16(2

**InchiKey:** MDOVKFQFZBKZGA-UHFFFAOYSA-N

**Formula:** C20H28BrFO4

**SMILES:** CCCCCCCCC(C)OC(=O)CCC(=O)Oc1ccc(F)cc1Br

**Mol. weight [g/mol]:** 431.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -440.10 | kJ/mol | Joback Method |
| hf | -907.20 | kJ/mol | Joback Method |
| hfus | 51.23 | kJ/mol | Joback Method |
| hvap | 87.26 | kJ/mol | Joback Method |
| log10ws | -7.28 | | Crippen Method |
| logp | 5.956 | | Crippen Method |
| mcvol | 303.050 | ml/mol | McGowan Method |
| pc | 1358.63 | kPa | Joback Method |
| rinpol | 2570.00 | | NIST Webbook |
| rinpol | 2570.00 | | NIST Webbook |
| tb | 911.21 | K | Joback Method |
| tc | 1121.61 | K | Joback Method |
| tf | 556.33 | K | Joback Method |
| vc | 1.169 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 924.82 | J/mol×K | 911.21 | Joback Method |
| cpg | 938.91 | J/mol×K | 946.28 | Joback Method |
| cpg | 951.84 | J/mol×K | 981.34 | Joback Method |
| cpg | 963.65 | J/mol×K | 1016.41 | Joback Method |
| cpg | 974.36 | J/mol×K | 1051.48 | Joback Method |
| cpg | 984.01 | J/mol×K | 1086.55 | Joback Method |
| cpg | 992.62 | J/mol×K | 1121.61 | 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=U389772&Units=SI |

# 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 |