# Succinic acid, 4-bromo-2,6-difluorobenzyl ethyl ester

**Inchi:** InChI=1S/C13H13BrF2O4/c1-2-19-12(17)3-4-13(18)20-7-9-10(15)5-8(14)6-11(9)16/h5-6
**InchiKey:** ZWDFVAXBVABPDC-UHFFFAOYSA-N
**Formula:** C13H13BrF2O4
**SMILES:** CCOC(=O)CCC(=O)OCc1c(F)cc(Br)cc1F
**Mol. weight [g/mol]:** 351.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -701.04 | kJ/mol | Joback Method |
| hf | -965.02 | kJ/mol | Joback Method |
| hfus | 39.32 | kJ/mol | Joback Method |
| hvap | 71.91 | kJ/mol | Joback Method |
| log10ws | -4.41 | | Crippen Method |
| logp | 3.114 | | Crippen Method |
| mcvol | 206.190 | ml/mol | McGowan Method |
| pc | 2248.26 | kPa | Joback Method |
| rinpol | 1947.00 | | NIST Webbook |
| rinpol | 1947.00 | | NIST Webbook |
| tb | 755.74 | K | Joback Method |
| tc | 960.90 | K | Joback Method |
| tf | 505.55 | K | Joback Method |
| vc | 0.801 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 537.23 | J/mol×K | 755.74 | Joback Method |
| cpg | 548.45 | J/mol×K | 789.93 | Joback Method |
| cpg | 558.91 | J/mol×K | 824.13 | Joback Method |
| cpg | 568.60 | J/mol×K | 858.32 | Joback Method |
| cpg | 577.52 | J/mol×K | 892.51 | Joback Method |
| cpg | 585.68 | J/mol×K | 926.70 | Joback Method |
| cpg | 593.08 | J/mol×K | 960.90 | Joback Method |

# Sources

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|---|---|
| **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=U381151&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 |