

# Succinic acid, 2-bromo-4-fluorophenyl 2-chloroethyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C12H11BrClFO4/c13-9-7-8(15)1-2-10(9)19-12(17)4-3-11(16)18-6-5-14/h1-2,7H |
| <b>InchiKey:</b>            | IFWQYAGKTGLKTB-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H11BrClFO4   |
| <b>SMILES:</b>              | O=C(CCC(=O)Oc1ccc(F)cc1Br)OCCCl   |
| <b>Mol. weight [g/mol]:</b> | 353.57  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -516.95 | kJ/mol               | Joback Method  |
| hf            | -752.54 | kJ/mol               | Joback Method  |
| hfus          | 38.23   | kJ/mol               | Joback Method  |
| hvap          | 74.22   | kJ/mol               | Joback Method  |
| log10ws       | -3.97   |                      | Crippen Method |
| logp          | 3.056   |                      | Crippen Method |
| mcvol         | 202.570 | ml/mol               | McGowan Method |
| pc            | 2525.19 | kPa                  | Joback Method  |
| rinsol        | 2158.00 |                      | NIST Webbook   |
| tb            | 766.04  | K                    | Joback Method  |
| tc            | 983.59  | K                    | Joback Method  |
| tf            | 511.09  | K                    | Joback Method  |
| vc            | 0.776   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 500.67 | J/mol×K | 766.04          | Joback Method |
| cpg           | 510.99 | J/mol×K | 802.30          | Joback Method |
| cpg           | 520.50 | J/mol×K | 838.56          | Joback Method |
| cpg           | 529.21 | J/mol×K | 874.82          | Joback Method |
| cpg           | 537.13 | J/mol×K | 911.07          | Joback Method |
| cpg           | 544.27 | J/mol×K | 947.33          | Joback Method |
| cpg           | 550.64 | J/mol×K | 983.59          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358012&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358012&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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