

# Terephthalic acid, 2-bromo-5-fluorobenzyl propyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C18H16BrFO4/c1-2-9-23-17(21)12-3-5-13(6-4-12)18(22)24-11-14-10-15(20)7- |
| <b>InchiKey:</b>            | BNNHOTYCXQJOIJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C18H16BrFO4  |
| <b>SMILES:</b>              | CCCOC(=O)c1ccc(C(=O)OCc2cc(F)ccc2Br)cc1  |
| <b>Mol. weight [g/mol]:</b> | 395.22   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -351.72 | kJ/mol               | Joback Method  |
| hf            | -635.58 | kJ/mol               | Joback Method  |
| hfus          | 43.23   | kJ/mol               | Joback Method  |
| hvap          | 86.13   | kJ/mol               | Joback Method  |
| log10ws       | -6.40   |                      | Crippen Method |
| logp          | 4.512   |                      | Crippen Method |
| mvol          | 251.110 | ml/mol               | McGowan Method |
| pc            | 2041.91 | kPa                  | Joback Method  |
| rinpol        | 2720.00 |                      | NIST Webbook   |
| rinpol        | 2720.00 |                      | NIST Webbook   |
| tb            | 897.55  | K                    | Joback Method  |
| tc            | 1129.47 | K                    | Joback Method  |
| tf            | 587.73  | K                    | Joback Method  |
| vc            | 0.956   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 705.53 | J/mol×K | 897.55          | Joback Method |
| cpg           | 716.83 | J/mol×K | 936.20          | Joback Method |
| cpg           | 726.98 | J/mol×K | 974.86          | Joback Method |
| cpg           | 736.00 | J/mol×K | 1013.51         | Joback Method |
| cpg           | 743.92 | J/mol×K | 1052.16         | Joback Method |
| cpg           | 750.77 | J/mol×K | 1090.82         | Joback Method |
| cpg           | 756.59 | J/mol×K | 1129.47         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416064&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416064&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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