

# Diglycolic acid, 2-bromo-4-fluorophenyl hexyl ester

|                             |                                                                                   |
|-----------------------------|-----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C16H20BrFO5/c1-2-3-4-5-8-22-15(19)10-21-11-16(20)23-14-7-6-12(18)9-13(1) |
| <b>InchiKey:</b>            | OPIZLRTUGASXAS-UHFFFAOYSA-N                                                       |
| <b>Formula:</b>             | C16H20BrFO5                                                                       |
| <b>SMILES:</b>              | CCCCCOC(=O)COCC(=O)Oc1ccc(F)cc1Br                                                 |
| <b>Mol. weight [g/mol]:</b> | 391.23                                                                            |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -576.34 | kJ/mol               | Joback Method  |
| hf            | -951.58 | kJ/mol               | Joback Method  |
| hfus          | 45.59   | kJ/mol               | Joback Method  |
| hvap          | 81.15   | kJ/mol               | Joback Method  |
| log10ws       | -4.58   |                      | Crippen Method |
| logp          | 3.634   |                      | Crippen Method |
| mvol          | 252.560 | ml/mol               | McGowan Method |
| pc            | 1804.63 | kPa                  | Joback Method  |
| rinpol        | 3075.00 |                      | NIST Webbook   |
| rinpol        | 3075.00 |                      | NIST Webbook   |
| tb            | 842.55  | K                    | Joback Method  |
| tc            | 1049.35 | K                    | Joback Method  |
| tf            | 548.48  | K                    | Joback Method  |
| vc            | 0.970   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 720.79 | J/mol×K | 842.55          | Joback Method |
| cpg           | 733.35 | J/mol×K | 877.02          | Joback Method |
| cpg           | 744.88 | J/mol×K | 911.48          | Joback Method |
| cpg           | 755.40 | J/mol×K | 945.95          | Joback Method |
| cpg           | 764.91 | J/mol×K | 980.41          | Joback Method |
| cpg           | 773.40 | J/mol×K | 1014.88         | Joback Method |
| cpg           | 780.89 | J/mol×K | 1049.35         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381997&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381997&amp;Units=SI</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                                 |

Latest version available from:

<https://www.cheméo.com/cid/117-021-8/Diglycolic-acid-2-bromo-4-fluorophenyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-30 11:44:33.348044296 +0000 UTC m=+16766722.268621611.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.