

# 2-[2-(2-Butoxyethoxy)ethyl]ethyl 2,2,3,3,3-pentafluoropropanoate

Other names:

Triethylene glycol monobutyl ether, pentafluoropropionate

3,6,9-Trioxatridec-1-yl pentafluoropropionate

Inchi:

InChI=1S/C13H21F5O5/c1-2-3-4-20-5-6-21-7-8-22-9-10-23-11(19)12(14,15)13(16,17)18

InchiKey:

BGBKSDBHTNZZQA-UHFFFAOYSA-N

Formula:

C13H21F5O5

SMILES:

CCCCOCCOCCOCCOC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]:

352.29

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -1458.71 | kJ/mol               | Joback Method  |
| hf            | -1951.16 | kJ/mol               | Joback Method  |
| hfus          | 36.35    | kJ/mol               | Joback Method  |
| hvap          | 54.24    | kJ/mol               | Joback Method  |
| log10ws       | -2.37    |                      | Crippen Method |
| logp          | 2.577    |                      | Crippen Method |
| mcvol         | 227.930  | ml/mol               | McGowan Method |
| pc            | 1415.44  | kPa                  | Joback Method  |
| rinpol        | 1455.80  |                      | NIST Webbook   |
| rinpol        | 1455.80  |                      | NIST Webbook   |
| tb            | 630.28   | K                    | Joback Method  |
| tc            | 786.49   | K                    | Joback Method  |
| tf            | 382.91   | K                    | Joback Method  |
| vc            | 0.909    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 646.58 | J/molxK | 630.28          | Joback Method |
| cpg           | 660.77 | J/molxK | 656.32          | Joback Method |
| cpg           | 674.32 | J/molxK | 682.35          | Joback Method |
| cpg           | 687.24 | J/molxK | 708.39          | Joback Method |
| cpg           | 699.53 | J/molxK | 734.42          | Joback Method |
| cpg           | 711.20 | J/molxK | 760.46          | 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.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>                                     |
| <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=U351988&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U351988&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>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>rinpol:</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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