

# 2-(2-Ethoxyethoxy)ethyl 2,2,3,3,3-pentafluoropropanoate

|                      |                                                                                                     |
|----------------------|-----------------------------------------------------------------------------------------------------|
| Other names:         | Diethylene glycol monoethyl ether, pentafluoropropionate<br>3,6-Dioxaoct-1-yl pentafluoropropionate |
| Inchi:               | InChI=1S/C9H13F5O4/c1-2-16-3-4-17-5-6-18-7(15)8(10,11)9(12,13)14/h2-6H2,1H3                         |
| InchiKey:            | FQCCIXQOWKJORU-UHFFFAOYSA-N                                                                         |
| Formula:             | C9H13F5O4                                                                                           |
| SMILES:              | CCOCCOCCOC(=O)C(F)(F)C(F)(F)F                                                                       |
| Mol. weight [g/mol]: | 280.19                                                                                              |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -1387.39 | kJ/mol  | Joback Method  |
| hf            | -1736.38 | kJ/mol  | Joback Method  |
| hfus          | 24.80    | kJ/mol  | Joback Method  |
| hvap          | 42.93    | kJ/mol  | Joback Method  |
| log10ws       | -1.60    |         | Crippen Method |
| logp          | 1.780    |         | Crippen Method |
| mcvol         | 165.700  | ml/mol  | McGowan Method |
| pc            | 1963.07  | kPa     | Joback Method  |
| rinpol        | 1051.80  |         | NIST Webbook   |
| tb            | 516.34   | K       | Joback Method  |
| tc            | 670.67   | K       | Joback Method  |
| tf            | 315.60   | K       | Joback Method  |
| vc            | 0.667    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 420.63 | J/mol×K | 516.34          | Joback Method |
| cpg           | 432.45 | J/mol×K | 542.06          | Joback Method |
| cpg           | 443.77 | J/mol×K | 567.78          | Joback Method |
| cpg           | 454.58 | J/mol×K | 593.50          | Joback Method |
| cpg           | 464.90 | J/mol×K | 619.22          | Joback Method |
| cpg           | 474.74 | J/mol×K | 644.95          | Joback Method |
| cpg           | 484.11 | J/mol×K | 670.67          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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=U351984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U351984&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>rlnpol:</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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