

# 2-(2-(2-(2-(2-Pentoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxy-trifluoroacetate

InChI: CCCCOCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F  
InChIKey: OVVKCIIGIGGYDY-UHFFFAOYSA-N

Formula: C<sub>19</sub>H<sub>35</sub>F<sub>3</sub>O<sub>8</sub>

SMILES: CCCCCOCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]: 448.47

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -1336.41 | kJ/mol               | Joback Method  |
| hf            | -2070.69 | kJ/mol               | Joback Method  |
| hfus          | 56.71    | kJ/mol               | Joback Method  |
| hvap          | 77.76    | kJ/mol               | Joback Method  |
| log10ws       | -1.82    |                      | Crippen Method |
| logp          | 2.382    |                      | Crippen Method |
| mcvol         | 326.540  | ml/mol               | McGowan Method |
| pc            | 968.07   | kPa                  | Joback Method  |
| rinpol        | 2366.10  |                      | NIST Webbook   |
| rinpol        | 2366.10  |                      | NIST Webbook   |
| tb            | 839.51   | K                    | Joback Method  |
| tc            | 1028.90  | K                    | Joback Method  |
| tf            | 513.62   | K                    | Joback Method  |
| vc            | 1.274    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1064.89 | J/mol×K | 839.51          | Joback Method |
| cpg           | 1082.57 | J/mol×K | 871.07          | Joback Method |
| cpg           | 1098.91 | J/mol×K | 902.64          | Joback Method |
| cpg           | 1113.90 | J/mol×K | 934.20          | Joback Method |
| cpg           | 1127.54 | J/mol×K | 965.77          | Joback Method |
| cpg           | 1139.79 | J/mol×K | 997.33          | Joback Method |
| cpg           | 1150.64 | J/mol×K | 1028.90         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=R188215&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R188215&amp;Units=SI</a> |
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rlnol:</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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