

# Glutaric acid, pentyl 2-(trifluoromethyl)benzyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C18H23F3O4/c1-2-3-6-12-24-16(22)10-7-11-17(23)25-13-14-8-4-5-9-15(14)18 |
| InchiKey:            | YSXCPCJXJKKYLD-UHFFFAOYSA-N  |
| Formula:             | C18H23F3O4   |
| SMILES:              | CCCCCOC(=O)CCCC(=O)OCc1ccccc1C(F)(F)F  |
| Mol. weight [g/mol]: | 360.37   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -845.97  | kJ/mol               | Joback Method  |
| hf            | -1276.47 | kJ/mol               | Joback Method  |
| hfus          | 43.43    | kJ/mol               | Joback Method  |
| hvap          | 73.17    | kJ/mol               | Joback Method  |
| log10ws       | -5.37    |                      | Crippen Method |
| logp          | 4.652    |                      | Crippen Method |
| mvol          | 260.910  | ml/mol               | McGowan Method |
| pc            | 1419.71  | kPa                  | Joback Method  |
| rinpol        | 2320.00  |                      | NIST Webbook   |
| tb            | 790.06   | K                    | Joback Method  |
| tc            | 980.80   | K                    | Joback Method  |
| tf            | 480.07   | K                    | Joback Method  |
| vc            | 1.026    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 785.53 | J/mol×K | 790.06          | Joback Method |
| cpg           | 799.99 | J/mol×K | 821.85          | Joback Method |
| cpg           | 813.48 | J/mol×K | 853.64          | Joback Method |
| cpg           | 826.05 | J/mol×K | 885.43          | Joback Method |
| cpg           | 837.71 | J/mol×K | 917.22          | Joback Method |
| cpg           | 848.52 | J/mol×K | 949.01          | Joback Method |
| cpg           | 858.49 | J/mol×K | 980.80          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U377491&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377491&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.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>                                     |

# 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>h vap:</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>m cvol:</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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