

# 4(1,1-Dimethylhexyl)phenol, pentafluorobenzoyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C21H21F5O2/c1-4-5-6-11-21(2,3)12-7-9-13(10-8-12)28-20(27)14-15(22)17(24) |
| <b>InchiKey:</b>            | WXDPLBRFRILNJ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C21H21F5O2  |
| <b>SMILES:</b>              | CCCCC(C)(C)c1ccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)cc1                                  |
| <b>Mol. weight [g/mol]:</b> | 400.38  |

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -912.15  | kJ/mol  | Joback Method  |
| hf            | -1306.63 | kJ/mol  | Joback Method  |
| hfus          | 46.67    | kJ/mol  | Joback Method  |
| hvap          | 74.64    | kJ/mol  | Joback Method  |
| log10ws       | -8.20    |         | Crippen Method |
| logp          | 6.459    |         | Crippen Method |
| mcvol         | 275.520  | ml/mol  | McGowan Method |
| pc            | 1255.70  | kPa     | Joback Method  |
| rinpol        | 2107.60  |         | NIST Webbook   |
| rinpol        | 2107.60  |         | NIST Webbook   |
| rinpol        | 2114.20  |         | NIST Webbook   |
| rinpol        | 2121.30  |         | NIST Webbook   |
| tb            | 832.53   | K       | Joback Method  |
| tc            | 1031.99  | K       | Joback Method  |
| tf            | 531.92   | K       | Joback Method  |
| vc            | 1.099    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 830.06 | J/molxK | 832.53          | Joback Method |
| cpg           | 844.22 | J/molxK | 865.77          | Joback Method |
| cpg           | 857.39 | J/molxK | 899.02          | Joback Method |
| cpg           | 869.62 | J/molxK | 932.26          | Joback Method |
| cpg           | 880.95 | J/molxK | 965.50          | Joback Method |
| cpg           | 891.41 | J/molxK | 998.74          | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=R433268&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R433268&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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