

# 2-Methylbenzene-1,4-diamine, N1,N1,N4,N4-tetrakis(pentafluoropropionyl)-

Other names: 2,5-Bis-di-pentafluoropropionylaminotoluene  
Inchi: InChI=1S/C19H6F20N2O4/c1-5-4-6(40(8(42)12(20,21)16(28,29)30)9(43)13(22,23)17(31)14(24,25)18(32,33)26(34,35)27(36,37)28)/p1/s1  
InchiKey: ORJZUETUVQYPGG-UHFFFAOYSA-N  
Formula: C19H6F20N2O4  
SMILES: Cc1cc(N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F)ccc1N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F  
Mol. weight [g/mol]: 706.23

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -3965.35 | kJ/mol  | Joback Method  |
| hf            | -4529.36 | kJ/mol  | Joback Method  |
| hfus          | 52.95    | kJ/mol  | Joback Method  |
| hvap          | 65.85    | kJ/mol  | Joback Method  |
| log10ws       | -8.12    |         | Crippen Method |
| logp          | 6.505    |         | Crippen Method |
| mcvol         | 316.450  | ml/mol  | McGowan Method |
| pc            | 952.01   | kPa     | Joback Method  |
| rinpol        | 1205.00  |         | NIST Webbook   |
| tb            | 870.68   | K       | Joback Method  |
| tc            | 1070.75  | K       | Joback Method  |
| tf            | 651.17   | K       | Joback Method  |
| vc            | 1.323    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1029.76 | J/mol×K | 870.68          | Joback Method |
| cpg           | 1038.32 | J/mol×K | 904.03          | Joback Method |
| cpg           | 1046.26 | J/mol×K | 937.37          | Joback Method |
| cpg           | 1053.80 | J/mol×K | 970.72          | Joback Method |
| cpg           | 1061.13 | J/mol×K | 1004.06         | Joback Method |
| cpg           | 1068.47 | J/mol×K | 1037.41         | Joback Method |
| cpg           | 1076.01 | J/mol×K | 1070.75         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U373219&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373219&amp;Units=SI</a> |
| <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>                     |

# 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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