

# Dichlofluanid

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Methanesulfenamide, 1,1-dichloro-N-[(dimethylamino)sulfonyl]-1-fluoro-N-phenyl-Sulfamide, N-[(dichlorofluoromethyl)thio]-N',N'-dimethyl-N-phenyl-Bayer 47531<br>BAY 47531<br>Dichlofluanide<br>Elvaron<br>Eparen<br>Euparen<br>Oiparen<br>Pecudin<br>N'-Dichlorofluoromethylthio-NN-dimethyl-N'-phenylsulphamide<br>Aniline, N-((dichlorofluoromethyl)thio)-N-((dimethylamino)sulfonyl)-Euparene<br>Ku 13-o32-c<br>KUE 13032c<br>N-(Dichlor-fluor-methyl-thio)-N',N'-dimethyl-N-phenyl-schwefel-saeurediamid<br>N-((Dichlorofluoromethyl)thio)-N',N'-dimethyl-N-phenylsulfamide<br>N,N-Dimethyl-N'-phenyl-N'-((fluorodichloromethyl)thio)sulfamide<br>1,1-Dichloro-N-((dimethylamino)sulfonyl)-1-fluoro-N-phenylmethanesulfenamide<br>Diclofluanide<br>NSC 218451 |
| <b>Inchi:</b>               | InChI=1S/C9H11Cl2FN2O2S2/c1-13(2)18(15,16)14(17-9(10,11)12)8-6-4-3-5-7-8/h3-7H,1  |
| <b>InchiKey:</b>            | WURGXGVFSMYFCG-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C9H11Cl2FN2O2S2   |
| <b>SMILES:</b>              | CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 333.23  |
| <b>CAS:</b>                 | 1085-98-9   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| gf            | -292.38 | kJ/mol | Joback Method  |
| hf            | -505.32 | kJ/mol | Joback Method  |
| hfus          | 38.72   | kJ/mol | Joback Method  |
| hvap          | 74.10   | kJ/mol | Joback Method  |
| log10ws       | -3.81   |        | Crippen Method |
| logp          | 3.006   |        | Crippen Method |

|        |         |                      |                |
|--------|---------|----------------------|----------------|
| mvol   | 204.560 | ml/mol               | McGowan Method |
| pc     | 3530.46 | kPa                  | Joback Method  |
| rinpol | 1947.00 |                      | NIST Webbook   |
| rinpol | 1965.00 |                      | NIST Webbook   |
| rinpol | 1921.00 |                      | NIST Webbook   |
| rinpol | 1943.00 |                      | NIST Webbook   |
| tb     | 644.34  | K                    | Joback Method  |
| tc     | 868.70  | K                    | Joback Method  |
| tf     | 418.36  | K                    | Joback Method  |
| vc     | 0.752   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 480.08 | J/mol×K | 644.34          | Joback Method |
| cpg           | 493.20 | J/mol×K | 681.73          | Joback Method |
| cpg           | 505.11 | J/mol×K | 719.13          | Joback Method |
| cpg           | 515.86 | J/mol×K | 756.52          | Joback Method |
| cpg           | 525.53 | J/mol×K | 793.91          | Joback Method |
| cpg           | 534.16 | J/mol×K | 831.31          | Joback Method |
| cpg           | 541.84 | J/mol×K | 868.70          | Joback Method |

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1085989&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>m<sub>cvol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>                 | Critical Pressure                               |
| <b>r<sub>inpol</sub>:</b>             | Non-polar retention indices                     |
| <b>t<sub>b</sub>:</b>                 | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>                 | Critical Temperature                            |
| <b>t<sub>f</sub>:</b>                 | Normal melting (fusion) point                   |
| <b>v<sub>c</sub>:</b>                 | Critical Volume                                 |

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