

# 9,9-Fluorenedipropionitrile

|                      |                                                                                                                                                                                                                                                     |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 9,9'-Fluorenedipropionitrile<br>9,9-Fluorenedipropionitrile<br>9H-Fluorene-9,9-dipropanenitrile<br>9H-fluorene-9,9-dipropiononitrile<br>Fluorene-9,9-bis(propionitrile)<br>Fluorene-9,9-dipropionitrile<br>Propionitrile, 3,3'-fluoren-9-ylidenedi- |
| Inchi:               | InChI=1S/C19H16N2/c20-13-5-11-19(12-6-14-21)17-9-3-1-7-15(17)16-8-2-4-10-18(16)19                                                                                                                                                                   |
| InchiKey:            | COWHDUMHYFLLER-UHFFFAOYSA-N                                                                                                                                                                                                                         |
| Formula:             | C19H16N2                                                                                                                                                                                                                                            |
| SMILES:              | N#CCCC1(CCC#N)c2ccccc2-c2ccccc21                                                                                                                                                                                                                    |
| Mol. weight [g/mol]: | 272.35                                                                                                                                                                                                                                              |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hfus          | 31.32   | kJ/mol | Joback Method  |
| logp          | 4.561   |        | Crippen Method |
| mcvol         | 222.950 | ml/mol | McGowan Method |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 654.65 | J/mol×K | 900.04          | Joback Method |
| cpg           | 670.07 | J/mol×K | 941.33          | Joback Method |
| cpg           | 685.98 | J/mol×K | 982.62          | Joback Method |
| cpg           | 702.66 | J/mol×K | 1023.91         | Joback Method |
| cpg           | 720.39 | J/mol×K | 1065.20         | Joback Method |
| cpg           | 739.45 | J/mol×K | 1106.49         | Joback Method |
| cpg           | 760.11 | J/mol×K | 1147.79         | 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>Cheméo Relay (1.0):</b>       |                                                                                                                                             |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                             |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4425972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4425972&amp;Units=SI</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>hfus:</b>  | Enthalpy of fusion at standard conditions |
| <b>logp:</b>  | Octanol/Water partition coefficient       |
| <b>mcvol:</b> | McGowan's characteristic volume           |

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