

3,5-Bis(trifluoromethyl)pyrazol

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|-----------------------------|---|
| Other names: | 3,3-Bis(trifluoromethyl)pyrazol 3,5-bis(trifluoromethyl)pyrazole |
| Inchi: | InChI=1S/C5H2F6N2/c6-4(7,8)2-1-3(13-12-2)5(9,10)11/h1H,(H,12,13) |
| InchiKey: | NGDDUAYSWPUSLX-UHFFFAOYSA-N |
| Formula: | C5H2F6N2 |
| SMILES: | FC(F)(F)c1cc(C(F)(F)F)[nH]n1 |
| Mol. weight [g/mol]: | 204.07 |
| CAS: | 14704-41-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -2.66 | | Crippen Method |
| logp | 1.965 | | Crippen Method |
| mcvol | 92.430 | ml/mol | McGowan Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------------|--------|-----------------|--------------|
| hsubt | 69.00 ± 0.60 | kJ/mol | 266.00 | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14704417&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|--|
| hsubt: | Enthalpy of sublimation at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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