

2,4,6-Tris(trichloromethyl)pyridine

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C8H2Cl9N/c9-6(10,11)3-1-4(7(12,13)14)18-5(2-3)8(15,16)17/h1-2H |
| InchiKey: | ZKYACIXSMBGRQP-UHFFFAOYSA-N |
| Formula: | C8H2Cl9N |
| SMILES: | <chem>C1C(Cl)(Cl)C1cc(C(Cl)(Cl)Cl)nc(C(Cl)(Cl)Cl)c1</chem> |
| Mol. weight [g/mol]: | 431.19 |
| CAS: | 6969-50-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.25 | | Crippen Method |
| logp | 6.562 | | Crippen Method |
| mcvol | 219.960 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6969502&Units=SI |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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