

5-Chloro-2-thiophenecarboxylic acid

| | |
|-----------------------------|--|
| Other names: | 5-Chlorothiophene-2-carboxylic acid 2-Thiophenecarboxylic acid, 5-chloro- 5-CHLORO-THIOPHENE-2-CARBOXILIC ACID |
| Inchi: | InChI=1S/C5H3ClO2S/c6-4-2-1-3(9-4)5(7)8/h1-2H,(H,7,8) |
| InchiKey: | QZLSBOVWPHXCLT-UHFFFAOYSA-N |
| Formula: | C5H3ClO2S |
| SMILES: | O=C(O)c1ccc(Cl)s1 |
| Mol. weight [g/mol]: | 162.59 |
| CAS: | 24065-33-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -1.97 | | Crippen Method |
| logp | 2.100 | | Crippen Method |
| mcvol | 97.880 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C24065336&Units=SI |
| 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 |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/63-470-0/5-Chloro-2-thiophenecarboxylic-acid.pdf>

Generated by Cheméo on 2024-05-01 00:09:13.89187933 +0000 UTC m=+16811402.812456645.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.