

3-Methylbenzo[b]thiophene-2-carboxaldehyde

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C10H8OS/c1-7-8-4-2-3-5-9(8)12-10(7)6-11/h2-6H,1H3 |
| InchiKey: | DRZGHNXLEQHVHB-UHFFFAOYSA-N |
| Formula: | C10H8OS |
| SMILES: | Cc1c(C=O)sc2ccccc12 |
| Mol. weight [g/mol]: | 176.24 |
| CAS: | 22053-74-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.75 | | Crippen Method |
| logp | 3.022 | | Crippen Method |
| mcvol | 130.760 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22053743&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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/13-263-5/3-Methylbenzo-b-thiophene-2-carboxaldehyde.pdf>

Generated by Cheméo on 2024-04-26 16:05:46.881025431 +0000 UTC m=+16436795.801602742.

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