

2-Thiophenecarboxamide, N-propyl-

Inchi: InChI=1S/C8H11NOS/c1-2-5-9-8(10)7-4-3-6-11-7/h3-4,6H,2,5H2,1H3,(H,9,10)
InchiKey: ZJJYCXCPUAOXFI-UHFFFAOYSA-N
Formula: C8H11NOS
SMILES: CCCNC(=O)c1cccs1
Mol. weight [g/mol]: 169.24

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.41 | | Crippen Method |
| logp | 1.888 | | Crippen Method |
| mcvol | 132.020 | ml/mol | McGowan Method |
| rinpol | 1571.00 | | NIST Webbook |
| rinpol | 1571.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407021&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/97-072-5/2-Thiophenecarboxamide-N-propyl.pdf>

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