# Furan, 2-hexyl-

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|---|---|
| **Other names:** | 2-Hexylfuran |
| | 2-n-Hexylfuran |
| **Inchi:** | InChI=1S/C10H16O/c1-2-3-4-5-7-10-8-6-9-11-10/h6,8-9H,2-5,7H2,1H3 |
| **InchiKey:** | XBLCAKKYMZVLPU-UHFFFAOYSA-N |
| **Formula:** | C10H16O |
| **SMILES:** | CCCCCCc1ccco1 |
| **Mol. weight [g/mol]:** | 152.23 |
| **CAS:** | 3777-70-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -7.68 | | Crippen Method |
| logp | 3.402 | | Crippen Method |
| mcvol | 138.170 | ml/mol | McGowan Method |
| rinpol | 1094.00 | | NIST Webbook |
| rinpol | 1097.00 | | NIST Webbook |
| rinpol | 1084.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1095.00 | | NIST Webbook |
| rinpol | 1094.00 | | NIST Webbook |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| rinpol | 1083.00 | | NIST Webbook |
| rinpol | 1086.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1080.00 | | NIST Webbook |
| rinpol | 1081.00 | | NIST Webbook |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1083.00 | | NIST Webbook |
| rinpol | 1097.00 | | NIST Webbook |
| ripol | 1329.00 | | NIST Webbook |
| ripol | 1345.00 | | NIST Webbook |
| ripol | 1326.00 | | NIST Webbook |
| ripol | 1345.00 | | NIST Webbook |
| ripol | 1318.00 | | NIST Webbook |
| ripol | 1323.00 | | NIST Webbook |
| ripol | 1316.00 | | NIST Webbook |

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|---|---|---|
| ripol | 1312.00 | NIST Webbook |
| ripol | 1312.00 | NIST Webbook |
| ripol | 1332.00 | NIST Webbook |
| ripol | 1329.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **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=C3777706&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |

Latest version available from:

https://www.chemeo.com/cid/46-384-5/Furan-2-hexyl.pdf

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