

Rose furan

| | |
|-----------------------------|--|
| Other names: | 2-(3-methyl-2-butenyl)-3-methylfuran 2-(3'-methyl-2'-butenyl)-3-methylfuran |
| Inchi: | InChI=1S/C10H14O/c1-8(2)4-5-10-9(3)6-7-11-10/h4,6-7H,5H2,1-3H3 |
| InchiKey: | UTSGPHXOHJSDBC-UHFFFAOYSA-N |
| Formula: | C10H14O |
| SMILES: | <chem>CC(C)=CCc1occc1C</chem> |
| Mol. weight [g/mol]: | 150.22 |
| CAS: | 15186-51-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.59 | | Crippen Method |
| logp | 3.097 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| rinpol | 1093.00 | | NIST Webbook |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1095.00 | | NIST Webbook |
| rinpol | 1065.00 | | NIST Webbook |
| rinpol | 1065.00 | | NIST Webbook |
| rinpol | 1087.00 | | NIST Webbook |
| rinpol | 1099.00 | | NIST Webbook |
| rinpol | 1104.30 | | NIST Webbook |
| rinpol | 1093.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| ripol | 1375.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1412.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1400.00 | | NIST Webbook |
| ripol | 1413.00 | | 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=C15186513&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/79-724-1/Rose-furan.pdf>

Generated by Cheméo on 2025-12-05 19:15:39.653125292 +0000 UTC m=+4710337.183165956.

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