

2-ethylthiofuran

Inchi: InChI=1S/C6H8OS/c1-2-8-6-4-3-5-7-6/h3-5H,2H2,1H3
InchiKey: CGCOPLAFHQVQEL-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CCSc1ccco1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	2.392		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R155983&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/18-635-7/2-ethylthiofuran.pdf>

Generated by Cheméo on 2024-04-29 23:16:20.934430348 +0000 UTC m=+16721829.855007675.

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