

Thiophene, 2-methyl-5-pentyl

Other names:	2-Methyl-5-pentylthiophene
Inchi:	InChI=1S/C10H16S/c1-3-4-5-6-10-8-7-9(2)11-10/h7-8H,3-6H2,1-2H3
InchiKey:	SAQLTJYOYWUZSD-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CCCCCc1ccc(C)s1
Mol. weight [g/mol]:	168.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	3.789		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
rinpola	1237.00		NIST Webbook
rinpola	1237.00		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=R41847&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/79-634-1/Thiophene-2-methyl-5-pentyl.pdf>

Generated by Cheméo on 2024-04-27 17:20:38.703918634 +0000 UTC m=+16527687.624495949.

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