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
rinpol	1237.00		NIST Webbook
rinpol	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/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