

Thiophene, 3-phenyl-

Other names:	3-Phenylthiophene
Inchi:	InChI=1S/C10H8S/c1-2-4-9(5-3-1)10-6-7-11-8-10/h1-8H
InchiKey:	ZDQZVKVIYAPRON-UHFFFAOYSA-N
Formula:	C10H8S
SMILES:	<chem>c1ccc(-c2ccsc2)cc1</chem>
Mol. weight [g/mol]:	160.24
CAS:	2404-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.415		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
ripol	1377.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	1377.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2140.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2090.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2404877&Units=SI

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

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