Thiophene, 2-phenyl-

Other names: 2-Phenylthiophene
Inchi: InChI=1S/C10H8S/c1-2-5-9(6-3-1)10-7-4-8-11-10/h1-8H
InchiKey: PJRGDKFLFAYRBV-UHFFFAOYSA-N
Formula: C10H8S
SMILES: c1ccc(-c2cccs2)cc1
Mol. weight [g/mol]: 160.24
CAS: 825-55-8

Physical Properties

Property code	Value	Unit	Source
ie	8.06	eV	NIST Webbook
log10ws	-3.83		Crippen Method
logp	3.415		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
rinpol	1376.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	2124.00		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=C825558&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
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