Thiophene, 2,5-diiodo-

Other names: 2,5-Diiodothiophene
Inchi: InChI=1S/C4H2I2S/c5-3-1-2-4(6)7-3/h1-2H
InchiKey: PNYWRAHWEIOAGK-UHFFFAOYSA-N
Formula: C4H2I2S
SMILES: Ic1ccc(I)s1
Mol. weight [g/mol]: 335.93
CAS: 625-88-7

Physical Properties

Property code	Value	Unit	Source
ie	8.35	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
ie	8.28	eV	NIST Webbook
log10ws	-3.53		Crippen Method
logp	2.957		Crippen Method
mcvol	115.750	ml/mol	McGowan Method
tb	412.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.70	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625887&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure