Thiophene, 2-propyl-

Other names:	2-Propylthiophene
	2-n-Propylthiophene
	isopropylthiophene
Inchi:	InChI=1S/C7H10S/c1-2-4-7-5-3-6-8-7/h3,5-6H,2,4H2,1H3
InchiKey:	BTXIJTYYMLCUHI-UHFFFAOYSA-N
Formula:	C7H10S
SMILES:	CCCc1cccs1
Mol. weight [g/mol]:	126.22
CAS:	1551-27-5

Physical Properties

Property code	Value	Unit	Source
hvap	43.70 ± 1.00	kJ/mol	NIST Webbook
ie	8.60 ± 0.20	eV	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.701		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	960.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	937.00		NIST Webbook
ripol	1259.00		NIST Webbook

ripol	1239.00		NIST Webbook
ripol	1238.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1259.00		NIST Webbook
tb	431.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	46.00	kJ/mol	273.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43889e+01
Coeff. B	-3.58516e+03
Coeff. C	-6.42650e+01
Temperature range (K), min.	318.51
Temperature range (K), max.	459.22

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1551275&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature