Thiophene, 2-(1,1-dimethylethyl)-

Other names:	2-tert-Butylthiophene
	Thiophene, 2-tert-butyl-
Inchi:	InChI=1S/C8H12S/c1-8(2,3)7-5-4-6-9-7/h4-6H,1-3H3
InchiKey:	SWCDOJGIOCVXFM-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CC(C)(C)c1cccs1
Mol. weight [g/mol]:	140.25
CAS:	1689-78-7

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	8.48	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	3.046		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
tb	437.10 ± 0.60	K	NIST Webbook
tf	214.00 ± 0.80	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52491e+01
Coeff. B	-3.98038e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	328.72
Temperature range (K), max.	463.22

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689787&Units=SI
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

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point