Thiophene, 3-(1,1-dimethylethyl)-

Other names:	3-(1,1-dimethylethyl) Thiophene
	3-tert-Butylthiophene
	Thiophene, 3-tert-butyl-
Inchi:	InChI=1S/C8H12S/c1-8(2,3)7-4-5-9-6-7/h4-6H,1-3H3
InchiKey:	LZDPZKBVRTYUMQ-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CC(C)(C)c1ccsc1
Mol. weight [g/mol]:	140.25
CAS:	1689-79-8

Physical Properties

Property code	Value	Unit	Source
ie	8.54 ± 0.05	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	3.046		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
tb	442.10 ± 1.00	K	NIST Webbook
tf	218.40 ± 0.80	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52552e+01
Coeff. B	-4.02108e+03
Coeff. C	-6.40680e+01
Temperature range (K), min.	332.72
Temperature range (K), max.	468.45

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1689798&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