Thiophene, 2-(1-methylethyl)-

Other names:	2-(1-Methylethyl)-thiophene
	2-Isopropylthiophene
	Isopropylthiophene
	Thiophene, 2-isopropyl-
Inchi:	InChI=1S/C7H10S/c1-6(2)7-4-3-5-8-7/h3-6H,1-2H3
InchiKey:	LOXBELRNKUFSRD-UHFFFAOYSA-N
Formula:	C7H10S
SMILES:	CC(C)c1cccs1
Mol. weight [g/mol]:	126.22
CAS:	4095-22-1

Physical Properties

Property code	Value	Unit	Source
chl	-4773.70 ± 1.80	kJ/mol	NIST Webbook
hfl	-11.60 ± 1.80	kJ/mol	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.871		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
rinpol	945.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	425.20 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	41.50	kJ/mol	410.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44373e+01
Coeff. B	-3.55428e+03
Coeff. C	-6.32200e+01
Temperature range (K), min.	314.41
Temperature range (K), max.	452.69

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4095221&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
hfl:	Liquid phase enthalpy of formation at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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