

Thiophene, 2-chloro-

Other names:	2-Chlorothiophene 2-Thienyl chloride
Inchi:	InChI=1S/C4H3ClS/c5-4-2-1-3-6-4/h1-3H
InchiKey:	GSFNQBFZFXUTBN-UHFFFAOYSA-N
Formula:	C4H3ClS
SMILES:	Clc1cccs1
Mol. weight [g/mol]:	118.58
CAS:	96-43-5

Physical Properties

Property code	Value	Unit	Source
ie	8.74 ± 0.04	eV	NIST Webbook
ie	8.89 ± 0.05	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.70 ± 0.05	eV	NIST Webbook
ie	9.06 ± 0.05	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
log10ws	-1.91		Crippen Method
logp	2.401		Crippen Method
mvol	76.350	ml/mol	McGowan Method
sl	209.11	J/molxK	NIST Webbook
tb	465.65 ± 1.50	K	NIST Webbook
tb	401.65 ± 1.50	K	NIST Webbook
tb	401.50	K	NIST Webbook
tt	201.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	139.43	J/molxK	298.15	NIST Webbook
hfust	8.97	kJ/mol	201.30	NIST Webbook
hfust	8.97	kJ/mol	201.30	NIST Webbook
hvapt	34.70	kJ/mol	357.00	NIST Webbook

hvapt	36.90	kJ/mol	360.50	NIST Webbook
hvapt	34.40	kJ/mol	353.50	NIST Webbook
sfust	44.54	J/molxK	201.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48221e+01
Coeff. B	-4.06128e+03
Coeff. C	-3.43100e+00
Temperature range (K), min.	282.85
Temperature range (K), max.	430.46

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96435&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions

tb: Normal Boiling Point Temperature

tt: Triple Point Temperature

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