

Thiophene, tetrachloro-

Other names:	2,3,4,5-Chlorothiophene 2,3,4,5-Tetrachlorothiophene ENT 25,764 IF IF (Fumigant) NSC 44615 NSC 61442 Pemphene Penn salt td-183 Penphene Perchlorothiophene TCTP TD-183 Tetrachlorothiofene Tetrachlorothiophene Tetrachlorthiofen Thiophene, 2,3,4,5-tetrachloro-
Inchi:	InChI=1S/C4Cl4S/c5-1-2(6)4(8)9-3(1)7
InchiKey:	WZXXZHONLFRKGG-UHFFFAOYSA-N
Formula:	C4Cl4S
SMILES:	Clc1sc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	221.92
CAS:	6012-97-1

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-3.97		Crippen Method
logp	4.362		Crippen Method
mcvol	113.070	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
---------------	-------	------	----------------	--------

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44935e+01
Coeff. B	-4.26179e+03
Coeff. C	-7.49760e+01
Temperature range (K), min.	374.98
Temperature range (K), max.	539.12

Sources

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=C6012971&Units=SI>

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tbrp:	Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/55-524-9/Thiophene-tetrachloro.pdf>

Generated by Cheméo on 2024-05-11 19:41:40.500821469 +0000 UTC m=+17745749.421398784.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.