

Thionyl chloride

Other names:	SOCI2 Sulfinyl chloride Sulfinyl dichloride Sulfur chloride oxide Sulfur chloride oxide (Cl2SO) Sulfur oxychloride Sulfur oxychloride (SOCl2) Sulfurous dichloride Sulfurous oxychloride Thionyl chloride (SOCl2) Thionyl dichloride UN 1836
Inchi:	InChI=1S/Cl2OS/c1-4(2)3
InchiKey:	FYSNRJHAOHDILO-UHFFFAOYSA-N
Formula:	Cl2OS
SMILES:	O=S(Cl)Cl
Mol. weight [g/mol]:	118.97
CAS:	7719-09-7

Physical Properties

Property code	Value	Unit	Source
gf	-292.45	kJ/mol	Joback Method
hf	-280.55	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	37.09	kJ/mol	Joback Method
ie	11.30	eV	NIST Webbook
ie	11.12	eV	NIST Webbook
ie	11.30	eV	NIST Webbook
ie	11.07	eV	NIST Webbook
ie	11.13	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	1.043		Crippen Method
mvol	57.560	ml/mol	McGowan Method
pc	6875.52	kPa	Joback Method
tb	332.54	K	Joback Method
tc	530.10	K	Joback Method
tf	186.08	K	Joback Method

vc

0.224

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	68.08	J/mol×K	332.54	Joback Method
cpg	69.47	J/mol×K	365.47	Joback Method
cpg	70.85	J/mol×K	398.39	Joback Method
cpg	72.21	J/mol×K	431.32	Joback Method
cpg	73.54	J/mol×K	464.24	Joback Method
cpg	74.83	J/mol×K	497.17	Joback Method
cpg	76.07	J/mol×K	530.10	Joback Method
hvapt	32.40	kJ/mol	314.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47469e+01
Coeff. B	-3.26001e+03
Coeff. C	-2.68900e+01
Temperature range (K), min.	172.00
Temperature range (K), max.	372.15

Sources

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>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7719097&Units=SI>

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvac:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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