Nitrosyl chloride

Other names:	NITROGEN CHLORIDE OXIDE
	NITROGEN OXIDE CHLORIDE
	NITROGEN OXYCHLORIDE
	NOCl
	Nitrogen chloride oxide (NOCl)
	Nitrogen oxide chloride (NOCl)
	Nitrogen oxychloride (NOCl)
	Nitrosonium chloride
	Nitrosyl chloride ((NO)Cl)
	ONCl
	UN 1069
Inchi:	InChI=1S/ClNO/c1-2-3
InchiKey:	VPCDQGACGWYTMC-UHFFFAOYSA-N
Formula:	ClNO
SMILES:	O=NCl
Mol. weight [g/mol]:	65.46
CAS:	2696-92-6

Physical Properties

Property code	Value	Unit	Source
dm	1.80	debye	KDB
gf	66.99	kJ/mol	KDB
hf	52.63	kJ/mol	KDB
hvap	29.08	kJ/mol	Joback Method
ie	10.90 ± 0.50	eV	NIST Webbook
ie	10.87 ± 0.01	eV	NIST Webbook
ie	10.94	eV	NIST Webbook
ie	12.70	eV	NIST Webbook
ie	10.90 ± 0.03	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	0.907		Crippen Method
mcvol	34.650	ml/mol	McGowan Method
pc	6170.82	kPa	Joback Method
tb	267.60	K	KDB
tc	440.00	K	KDB
tf	213.60	K	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	25.30	kJ/mol	230.50	NIST Webbook
rhol	1420.00	kg/m3	261.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60272e+01
Coeff. B	-3.02758e+03
Coeff. C	-2.40000e+00
Temperature range (K), min.	213.55
Temperature range (K), max.	440.65

Sources

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1897

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2696926&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

dm: Dipole Moment

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hvap:	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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point