Sulfuryl chloride fluoride

Other names:	Chloro fluoro sulfone
	Chlorosulfonyl fluoride
	Fluorosulfonyl chloride
	Fluorosulfuryl chloride
	SO2ClF
	SO2FCl
	Sulfonyl chloride fluoride
	Sulfuryl chlorofluoride
	Sulfuryl fluoride chloride
	Sulfuryl fluorochloride
	TL 212
	chlorosulphonyl fluoride
Inchi:	InChI=1S/ClFO2S/c1-5(2,3)4
InchiKey:	IXPAAHZTOUOJJM-UHFFFAOYSA-N
Formula:	ClFO2S
SMILES:	O=S(=O)(F)Cl
Mol. weight [g/mol]:	118.52
CAS:	13637-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-726.16	kJ/mol	Joback Method
hf	-708.53	kJ/mol	Joback Method
hfus	14.41	kJ/mol	Joback Method
hvap	37.80	kJ/mol	Joback Method
ie	12.40	eV	NIST Webbook
ie	12.61	eV	NIST Webbook
ie	12.30 ± 0.50	eV	NIST Webbook
log10ws	-0.64		Crippen Method
logp	0.440		Crippen Method
mcvol	52.960	ml/mol	McGowan Method
pc	7627.62	kPa	Joback Method
tb	283.88	K	Joback Method
tc	443.51	K	Joback Method
tf	158.83	K	Joback Method
vc	0.229	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	73.88	J/mol×K	283.88	Joback Method
cpg	75.77	J/mol×K	310.49	Joback Method
cpg	77.67	J/mol×K	337.09	Joback Method
cpg	79.55	J/mol×K	363.70	Joback Method
cpg	81.42	J/mol×K	390.30	Joback Method
cpg	83.26	J/mol×K	416.91	Joback Method
cpg	85.07	J/mol×K	443.51	Joback Method
hvapt	29.00	kJ/mol	255.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30013e+01
Coeff. B	-1.82763e+03
Coeff. C	-6.24500e+01
Temperature range (K), min.	201.00
Temperature range (K), max.	310.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13637848&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

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

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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume