Methanesulfenyl chloride, trifluoro-

Other names:	Perfluoromethylsulfenyl chloride
	Trifluoromethanesulfenyl chloride
	Trifluoromethylsulfenyl chloride
	trifluoromethanesulphenyl chloride
Inchi:	InChI=1S/CClF3S/c2-6-1(3,4)5
InchiKey:	RQYLOOVORNJDQX-UHFFFAOYSA-N
Formula:	CClF3S
SMILES:	FC(F)(F)SCl
Mol. weight [g/mol]:	136.52
CAS:	421-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-602.86	kJ/mol	Joback Method
hf	-634.92	kJ/mol	Joback Method
hfus	8.50	kJ/mol	Joback Method
hvap	25.28	kJ/mol	Joback Method
ie	10.70 ± 0.10	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	2.393		Crippen Method
mcvol	58.850	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	323.07	K	Joback Method
tc	504.54	K	Joback Method
tf	169.54	K	Joback Method
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.85	J/mol×K	323.07	Joback Method
cpg	94.74	J/mol×K	353.32	Joback Method
cpg	98.35	J/mol×K	383.56	Joback Method
cpg	101.68	J/mol×K	413.81	Joback Method

cpg	104.74	J/mol×K	444.05	Joback Method
cpg	107.56	J/mol×K	474.30	Joback Method
cpg	110.14	J/mol×K	504.54	Joback Method
hvapt	24.50	kJ/mol	259.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.21012e+01
Coeff. B	-1.47340e+03
Coeff. C	-7.56500e+01
Temperature range (K), min.	200.37
Temperature range (K), max.	292.66

Sources

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=C421170&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

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