

Methanesulfonyl chloride, trichloro-

Other names:	Trichloromethanesulfonyl chloride Trichloromethylsulfonyl chloride Trichloromethanesulphenyl chloride Trichloromethanesulphonyl chloride
Inchi:	InChI=1S/CCl4O2S/c2-1(3,4)8(5,6)7
InchiKey:	ZCPSWAFANXCCOT-UHFFFAOYSA-N
Formula:	CCl4O2S
SMILES:	O=S(=O)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	217.89
CAS:	2547-61-7

Physical Properties

Property code	Value	Unit	Source
gf	-555.88	kJ/mol	Joback Method
hf	-589.03	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.883		Crippen Method
mcvol	102.000	ml/mol	McGowan Method
pc	6027.93	kPa	Joback Method
rinpol	1024.00		NIST Webbook
rinpol	1035.00		NIST Webbook
tb	416.55	K	Joback Method
tc	629.11	K	Joback Method
tf	261.69	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.26	J/mol×K	593.69	Joback Method
cpg	146.58	J/mol×K	416.55	Joback Method
cpg	150.88	J/mol×K	451.98	Joback Method

cpg	154.78	J/mol×K	487.40	Joback Method
cpg	158.31	J/mol×K	522.83	Joback Method
cpg	161.47	J/mol×K	558.26	Joback Method
cpg	166.72	J/mol×K	629.11	Joback Method
hfust	7.46	kJ/mol	418.50	NIST Webbook

Sources

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=C2547617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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