TRIFLUOROMETHANESULFONYL CHLORIDE

Other names: Methanesulfonyl chloride, trifluoro-
trifluoromethanesulphonyl chloride
Inchi: InChI=1S/CClF3O2S/c2-8(6,7)1(3,4)5
InchiKey: GRGCWBWNLSTIEN-UHFFFAOYSA-N
Formula: CClF3O2S
SMILES: O=S(=O)(Cl)C(F)(F)F
Mol. weight [g/mol]: 168.52

Physical Properties

Property code	Value	Unit	Source
hfus	15.75	kJ/mol	Joback Method
ie	12.41	eV	Cheméo Relay (1.0)
logp	1.075		Crippen Method
mcvol	70.590	ml/mol	McGowan Method
tb	305.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.79	J/mol×K	302.07	Joback Method
cpg	119.40	J/mol×K	327.60	Joback Method
cpg	123.80	J/mol×K	353.13	Joback Method
cpg	127.97	J/mol×K	378.66	Joback Method
cpg	131.93	J/mol×K	404.19	Joback Method
cpg	135.67	J/mol×K	429.72	Joback Method
cpg	139.21	J/mol×K	455.24	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C421830&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature