2,3,4-Trichlorobenzenesulfonyl chloride

Other names: Benzenesulfonyl chloride, 2,3,4-trichloro-
2,3,4-trichlorobenzenesulphonyl chloride
Inchi: InChI=1S/C6H2Cl4O2S/c7-3-1-2-4(13(10,11)12)6(9)5(3)8/h1-2H
InchiKey: JDAJYNHGBUXIKS-UHFFFAOYSA-N
Formula: C6H2Cl4O2S
SMILES: O=S(=O)(Cl)c1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 279.96

Physical Properties

Property code	Value	Unit	Source
hf	-335.54	kJ/mol	Cheméo Relay (1.0)
hfus	32.34	kJ/mol	Joback Method
hvap	89.41	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-4.70		Cheméo Relay (1.0)
logp	3.574		Crippen Method
mcvol	148.690	ml/mol	McGowan Method
tb	590.77	K	Cheméo Relay (1.0)
tf	378.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.03	J/mol×K	575.80	Joback Method
cpg	263.19	J/mol×K	614.95	Joback Method
cpg	269.80	J/mol×K	654.09	Joback Method
cpg	275.86	J/mol×K	693.24	Joback Method
cpg	281.36	J/mol×K	732.39	Joback Method
cpg	286.30	J/mol×K	771.53	Joback Method
cpg	290.67	J/mol×K	810.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34732097&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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point