2,4-Dichlorobenzenesulfonyl chloride

Other names: 2,4-Dichlorobenzenesulfonyl chloride
Inchi: InChI=1S/C6H3Cl3O2S/c7-4-1-2-6(5(8)3-4)12(9,10)11/h1-3H
InchiKey: FDTPBIKNYWQLAE-UHFFFAOYSA-N
Formula: C6H3Cl3O2S
SMILES: O=S(=O)(Cl)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 245.51

Physical Properties

Property code	Value	Unit	Source
hf	-313.19	kJ/mol	Cheméo Relay (1.0)
hfus	28.53	kJ/mol	Joback Method
hvap	81.86	kJ/mol	Cheméo Relay (1.0)
ie	9.64	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	2.921		Crippen Method
mcvol	136.450	ml/mol	McGowan Method
tb	561.10	K	Cheméo Relay (1.0)
tf	335.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.72	J/mol×K	533.39	Joback Method
cpg	245.90	J/mol×K	571.64	Joback Method
cpg	253.51	J/mol×K	609.89	Joback Method
cpg	260.54	J/mol×K	648.15	Joback Method
cpg	267.00	J/mol×K	686.40	Joback Method
cpg	272.88	J/mol×K	724.65	Joback Method
cpg	278.19	J/mol×K	762.90	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16271333&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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