3-Chloro-4-fluorobenzenesulfonyl chloride

Inchi: InChI=1S/C6H3Cl2FO2S/c7-5-3-4(12(8,10)11)1-2-6(5)9/h1-3H
InchiKey: DXFXNSNBZNELII-UHFFFAOYSA-N
Formula: C6H3Cl2FO2S
SMILES: O=S(=O)(Cl)c1ccc(F)c(Cl)c1
Mol. weight [g/mol]: 229.06

Physical Properties

Property code	Value	Unit	Source
hfus	27.41	kJ/mol	Joback Method
ie	9.86	eV	Cheméo Relay (1.0)
logp	2.407		Crippen Method
mcvol	125.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.24	J/mol×K	495.23	Joback Method
cpg	233.59	J/mol×K	530.68	Joback Method
cpg	241.45	J/mol×K	566.12	Joback Method
cpg	248.81	J/mol×K	601.57	Joback Method
cpg	255.68	J/mol×K	637.02	Joback Method
cpg	262.05	J/mol×K	672.46	Joback Method
cpg	267.91	J/mol×K	707.91	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91170933&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

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