3-Chloro-2-Methylbenzenesulphonyl chloride

Inchi: InChI=1S/C7H6Cl2O2S/c1-5-6(8)3-2-4-7(5)12(9,10)11/h2-4H,1H3
InchiKey: ZSIYKAQPQRTBPF-UHFFFAOYSA-N
Formula: C7H6Cl2O2S
SMILES: Cc1c(Cl)cccc1S(=O)(=O)Cl
Mol. weight [g/mol]: 225.09
CAS: 80563-86-6

Physical Properties

Property code	Value	Unit	Source
gf	-391.19	kJ/mol	Joback Method
hf	-459.05	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.576		Crippen Method
mcvol	138.300	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	518.84	K	Joback Method
tc	739.50	K	Joback Method
tf	318.51	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.69	J/mol×K	518.84	Joback Method
cpg	267.76	J/mol×K	555.62	Joback Method
cpg	277.23	J/mol×K	592.39	Joback Method
cpg	286.09	J/mol×K	629.17	Joback Method
cpg	294.34	J/mol×K	665.94	Joback Method
cpg	301.99	J/mol×K	702.72	Joback Method
cpg	309.03	J/mol×K	739.50	Joback Method

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=C80563866&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume