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]: 225.10

Physical Properties

Property code	Value	Unit	Source
hfus	26.92	kJ/mol	Joback Method
logp	2.576		Crippen Method
mcvol	138.300	ml/mol	McGowan Method
tb	554.92	K	Cheméo Relay (1.0)
tf	364.14	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80563866&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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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