

4-Chlorobenzenesulfonyl isocyanate

Other names:	p-Chlorobenzenesulfonyl isocyanate
Inchi:	InChI=1S/C7H4ClNO3S/c8-6-1-3-7(4-2-6)13(11,12)9-5-10/h1-4H
InchiKey:	JGHDVROWMPBQSR-UHFFFAOYSA-N
Formula:	C7H4ClNO3S
SMILES:	O=C=NS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	217.63
CAS:	5769-15-3

Physical Properties

Property code	Value	Unit	Source
hf	-437.25	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	1.365		Crippen Method
mcvol	133.310	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	543.10	K	Joback Method
tc	765.56	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C5769153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation 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

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