

3,5-Dichlorobenzenesulfonyl chloride

Inchi:	InChI=1S/C6H3Cl3O2S/c7-4-1-5(8)3-6(2-4)12(9,10)11/h1-3H
InchiKey:	RJSQINMKOSOUGT-UHFFFAOYSA-N
Formula:	C6H3Cl3O2S
SMILES:	O=S(=O)(Cl)c1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	245.51
CAS:	705-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-411.54	kJ/mol	Joback Method
hf	-454.15	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	64.34	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.921		Crippen Method
mcvol	136.450	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	533.39	K	Joback Method
tc	762.90	K	Joback Method
tf	337.16	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.72	J/molxK	533.39	Joback Method
cpg	245.90	J/molxK	571.64	Joback Method
cpg	253.51	J/molxK	609.89	Joback Method
cpg	260.54	J/molxK	648.15	Joback Method
cpg	267.00	J/molxK	686.40	Joback Method
cpg	272.88	J/molxK	724.65	Joback Method
cpg	278.19	J/molxK	762.90	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=C705215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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