

2,4,6-Trichlorobenzenesulfonyl chloride

Inchi:	InChI=1S/C6H2Cl4O2S/c7-3-1-4(8)6(5(9)2-3)13(10,11)12/h1-2H
InchiKey:	WHJAQKAAIOHCGN-UHFFFAOYSA-N
Formula:	C6H2Cl4O2S
SMILES:	O=S(=O)(Cl)c1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	279.96
CAS:	51527-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-433.10	kJ/mol	Joback Method
hf	-481.36	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.574		Crippen Method
mcvol	148.690	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	575.80	K	Joback Method
tc	810.68	K	Joback Method
tf	379.60	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.03	J/molxK	575.80	Joback Method
cpg	263.19	J/molxK	614.95	Joback Method
cpg	269.80	J/molxK	654.09	Joback Method
cpg	275.86	J/molxK	693.24	Joback Method
cpg	281.36	J/molxK	732.39	Joback Method
cpg	286.30	J/molxK	771.53	Joback Method
cpg	290.67	J/molxK	810.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51527732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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