

Benzenesulfonyl chloride, 4-chloro-3-nitro-

Other names:	Yellow Sulfon Chloride 3-Nitro-4-chlorobenzenesulfonyl chloride 4-Chloro-3-nitrobenzenesulfonyl chloride 2-Chloro-1-nitrobenzene-5-sulfonyl chloride 4-chloro-3-nitrobenzenesulphonyl chloride
Inchi:	InChI=1S/C6H3Cl2NO4S/c7-5-2-1-4(14(8,12)13)3-6(5)9(10)11/h1-3H
InchiKey:	SEWNAJIUKSTYOP-UHFFFAOYSA-N
Formula:	C6H3Cl2NO4S
SMILES:	O=[N+]([O-])c1cc(S(=O)(=O)Cl)ccc1Cl
Mol. weight [g/mol]:	256.06
CAS:	97-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-364.06	kJ/mol	Joback Method
hf	-449.17	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	76.55	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.176		Crippen Method
mcvol	141.630	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	647.80	K	Joback Method
tc	898.69	K	Joback Method
tf	450.85	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.63	J/molxK	647.80	Joback Method
cpg	299.90	J/molxK	689.61	Joback Method
cpg	307.36	J/molxK	731.43	Joback Method
cpg	314.01	J/molxK	773.24	Joback Method

cpg	319.87	J/mol×K	815.06	Joback Method
cpg	324.92	J/mol×K	856.87	Joback Method
cpg	329.19	J/mol×K	898.69	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=C97085&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

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