

m-(Chlorosulfonyl)benzoic acid

Other names:	Benzoic acid, 3-(chlorosulfonyl)- Benzoic acid, m-(chlorosulfonyl)- 3-(Chlorosulfonyl)benzoic acid 3-Carboxybenzenesulfonyl chloride 3-Carboxyphenylsulfonyl chloride 3-(chlorosulphonyl)benzoic acid
Inchi:	InChI=1S/C7H5ClO4S/c8-13(11,12)6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	LMRKXSDOAFUINK-UHFFFAOYSA-N
Formula:	C7H5ClO4S
SMILES:	O=C(O)c1cccc(S(=O)(=O)Cl)c1
Mol. weight [g/mol]:	220.63
CAS:	4025-64-3

Physical Properties

Property code	Value	Unit	Source
gf	-635.37	kJ/mol	Joback Method
hf	-696.65	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.312		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	5908.07	kPa	Joback Method
tb	622.48	K	Joback Method
tc	829.71	K	Joback Method
tf	386.82	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.92	J/mol×K	622.48	Joback Method
cpg	295.95	J/mol×K	657.02	Joback Method
cpg	303.38	J/mol×K	691.56	Joback Method

cpg	310.22	J/mol×K	726.09	Joback Method
cpg	316.47	J/mol×K	760.63	Joback Method
cpg	322.14	J/mol×K	795.17	Joback Method
cpg	327.24	J/mol×K	829.71	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=C4025643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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