

Benzenamine, 4-chloro-N-sulfinyl-

Other names:	Aniline, p-chloro-N-sulfinyl- (p-Chlorophenyl)sulfinylamine p-Chloro-N-sulfinylaniline N-Sulfinyl-p-chloroaniline Thionyl-p-chloroaniline 4-Chlorosulfinylaniline p-Chloro-N-thionylaniline 4-Chloro-N-sulfinylbenzenamine 4-Chloro-N-sulfinylaniline
Inchi:	InChI=1S/C6H4ClNOS/c7-5-1-3-6(4-2-5)8-10-9/h1-4H
InchiKey:	GTKDDSPQJMLGOM-UHFFFAOYSA-N
Formula:	C6H4ClNOS
SMILES:	O=S=Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	173.62
CAS:	13165-68-9

Physical Properties

Property code	Value	Unit	Source
hf	-84.17	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	2.368		Crippen Method
mvol	111.780	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	537.95	K	Joback Method
tc	781.91	K	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=C13165689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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