

Benzenethiol, 3-chloro-

Other names:	Benzenethiol, m-chloro- m-Chlorobenzenethiol m-Chlorothiophenol 3-Chlorobenzenethiol 3-Chlorothiophenol
Inchi:	InChI=1S/C6H5ClS/c7-5-2-1-3-6(8)4-5/h1-4,8H
InchiKey:	CQJDYPZUDYXHLM-UHFFFAOYSA-N
Formula:	C6H5ClS
SMILES:	Sc1cccc(Cl)c1
Mol. weight [g/mol]:	144.62
CAS:	2037-31-2

Physical Properties

Property code	Value	Unit	Source
gf	119.88	kJ/mol	Joback Method
hf	80.63	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	43.01	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.629		Crippen Method
mcvol	100.230	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	479.20	K	NIST Webbook
tc	720.14	K	Joback Method
tf	262.70	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.41	J/mol×K	468.63	Joback Method
cpg	174.66	J/mol×K	510.55	Joback Method
cpg	183.22	J/mol×K	552.47	Joback Method
cpg	191.14	J/mol×K	594.38	Joback Method

cpg	198.44	J/mol×K	636.30	Joback Method
cpg	205.16	J/mol×K	678.22	Joback Method
cpg	211.34	J/mol×K	720.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	4.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2037312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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