

Benzenethiol, 2,5-dichloro-

Other names:	Thiophenol, 2,5-dichloro- 2,5-Dichlorobenzenethiol 2,5-Dichlorothiophenol
Inchi:	InChI=1S/C6H4Cl2S/c7-4-1-2-5(8)6(9)3-4/h1-3,9H
InchiKey:	QIULLHZMZMGGFH-UHFFFAOYSA-N
Formula:	C6H4Cl2S
SMILES:	Sc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	179.07
CAS:	5858-18-4

Physical Properties

Property code	Value	Unit	Source
gf	98.32	kJ/mol	Joback Method
hf	53.42	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.282		Crippen Method
mcvol	112.470	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	511.04	K	Joback Method
tc	769.63	K	Joback Method
tf	305.14	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.08	J/molxK	511.04	Joback Method
cpg	193.15	J/molxK	554.14	Joback Method
cpg	200.62	J/molxK	597.24	Joback Method
cpg	207.51	J/molxK	640.34	Joback Method
cpg	213.84	J/molxK	683.44	Joback Method
cpg	219.66	J/molxK	726.54	Joback Method

cpg

224.97

J/mol×K

769.63

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	6.70	NIST Webbook

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=C5858184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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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