2,3-DICHLOROBENZENETHIOL

Other names: 2,3-Dichlorothiophenol
Benzenethiol, 2,3-dichloro-
Inchi: InChI=1S/C6H4Cl2S/c7-4-2-1-3-5(9)6(4)8/h1-3,9H
InchiKey: QGRKONUHHGBHRB-UHFFFAOYSA-N
Formula: C6H4Cl2S
SMILES: Sc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 179.07

Physical Properties

Property code	Value	Unit	Source
af	0.3447		Cheméo Relay (1.0)
gf	98.32	kJ/mol	Joback Method
hf	32.63	kJ/mol	Cheméo Relay (1.0)
hfus	17.00	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Cheméo Relay (1.0)
ie	8.49	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)
logp	3.282		Crippen Method
mcvol	112.470	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	514.23	K	Cheméo Relay (1.0)
tc	783.00	K	Cheméo Relay (1.0)
tf	300.56	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	224.97	J/mol×K	769.63	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17231957&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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