Chlorthiamid

Other names:	2,6-Dichlorothiobenzamide
	Benzenecarbothioamide, 2,6-dichloro-
	Benzamide, 2,6-dichlorothio-
	Chlorothiamide
	Chlorthiamide
	Chlorthioamide
	Chlortiamid
	DCBN
	2,6-Dichlorobenzenecarbothioamide
	2,6-Dichlor-thiobenzamid
	Prefix
	SD 7961
	WL-5792
Inchi:	InChI=1S/C7H5Cl2NS/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H2,10,11)
InchiKey:	KGKGSIUWJCAFPX-UHFFFAOYSA-N
Formula:	C7H5Cl2NS
SMILES:	NC(=S)c1c(Cl)cccc1Cl
Mol. weight [g/mol]:	206.09
CAS:	1918-13-4

Physical Properties

Property code	Value	Unit	Source
gf	260.86	kJ/mol	Joback Method
hf	174.59	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.628		Crippen Method
mcvol	132.240	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	613.63	K	Joback Method
tc	880.36	K	Joback Method
tf	397.48	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.45	J/mol×K	613.63	Joback Method
cpg	260.32	J/mol×K	658.09	Joback Method
cpg	267.45	J/mol×K	702.54	Joback Method
cpg	273.94	J/mol×K	747.00	Joback Method
cpg	279.87	J/mol×K	791.45	Joback Method
cpg	285.36	J/mol×K	835.91	Joback Method
cpg	290.49	J/mol×K	880.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1918134&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume