2-Chlorothiobenzamide

Other names: Benzenecarbothioamide, 2-chloro-
Benzamide, o-chlorothio-
2-Chlorobenzenecarbothioamide
Inchi: InChI=1S/C7H6ClNS/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H2,9,10)
InchiKey: FLQYOORLPNYQEV-UHFFFAOYSA-N
Formula: C7H6ClNS
SMILES: NC(=S)c1ccccc1Cl
Mol. weight [g/mol]: 171.65
CAS: 15717-17-6

Physical Properties

Property code	Value	Unit	Source
gf	282.42	kJ/mol	Joback Method
hf	201.80	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-2.93		Crippen Method
logp	1.974		Crippen Method
mcvol	120.000	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	571.22	K	Joback Method
tc	833.59	K	Joback Method
tf	355.04	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.81	J/mol×K	571.22	Joback Method
cpg	243.97	J/mol×K	614.95	Joback Method
cpg	252.25	J/mol×K	658.68	Joback Method
cpg	259.76	J/mol×K	702.40	Joback Method
cpg	266.59	J/mol×K	746.13	Joback Method

cpg	272.84	J/mol×K	789.86	Joback Method
cpg	278.62	J/mol×K	833.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15717176&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

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
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