4-Chloro-meta-benzenedithiol

Other names: 1,3-Benzenedithiol, 4-chloro-
4-chlorobenzene-1,3-dithiol
Inchi: InChI=1S/C6H5ClS2/c7-5-2-1-4(8)3-6(5)9/h1-3,8-9H
InchiKey: HCDLDZCJYMCKQH-UHFFFAOYSA-N
Formula: C6H5ClS2
SMILES: Sc1ccc(Cl)c(S)c1
Mol. weight [g/mol]: 176.69
CAS: 58593-78-5

Physical Properties

Property code	Value	Unit	Source
gf	139.64	kJ/mol	Joback Method
hf	107.64	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.917		Crippen Method
mcvol	116.580	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	536.47	K	Joback Method
tc	815.10	K	Joback Method
tf	311.68	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.82	J/mol×K	536.47	Joback Method
cpg	210.80	J/mol×K	582.91	Joback Method
cpg	219.07	J/mol×K	629.35	Joback Method
cpg	226.65	J/mol×K	675.79	Joback Method
cpg	233.58	J/mol×K	722.22	Joback Method
cpg	239.89	J/mol×K	768.66	Joback Method
cpg	245.61	J/mol×K	815.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.70	K	1.70	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=C58593785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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