Halazone

Other names:	Benzoic acid, 4-[(dichloroamino)sulfonyl]-
	Benzoic acid, p-(dichlorosulfamoyl)-
	p-(N,N-Dichlorosulfamoyl)benzoic acid
	p-(N,N-Dichlorosulfamyl)benzoic acid
	p-Carboxybenzenesulfondichloroamide
	p-Dichlorosulfamoylbenzoic acid
	p-Sulfondichloramidobenzoic acid
	Halazon
	Pantocid
	Pantocide
	Pantosid
	Pantotsid
	Pentocid
	Zeptabs
	Cloritines
	Parasulfondichloramido benzoic acid
	4-(N,N-Dichlorosulfamoyl)benzoic acid
	Kyselina p-N,N-dichlorsulfamoylbenzoova
	NSC 60717
Inchi:	InChI=1S/C7H5Cl2NO4S/c8-10(9)15(13,14)6-3-1-5(2-4-6)7(11)12/h1-4H,(H,11,12)
InchiKey:	XPDVQPODLRGWPL-UHFFFAOYSA-N
Formula:	C7H5Cl2NO4S
SMILES:	O=C(O)c1ccc(S(=O)(=O)N(Cl)Cl)cc1
Mol. weight [g/mol]:	270.09
CAS:	80-13-7

Physical Properties

Property code	Value	Unit	Source
gf	-536.52	kJ/mol	Joback Method
hf	-644.86	kJ/mol	Joback Method
hfus	36.02	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.683		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	672.35	K	Joback Method

tc	880.47	K	Joback Method
tf	449.21	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.38	J/mol×K	672.35	Joback Method
cpg	351.04	J/mol×K	707.04	Joback Method
cpg	358.03	J/mol×K	741.72	Joback Method
cpg	364.35	J/mol×K	776.41	Joback Method
cpg	370.04	J/mol×K	811.09	Joback Method
cpg	375.09	J/mol×K	845.78	Joback Method
cpg	379.53	J/mol×K	880.47	Joback Method

Sources

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=C80137&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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