P-(N,N-DICHLOROSULFAMOYL)BENZOIC ACID

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

Physical Properties

Property code	Value	Unit	Source
af	0.7605		Cheméo Relay (1.0)
gf	-536.52	kJ/mol	Joback Method
hf	-406.34	kJ/mol	Cheméo Relay (1.0)
hfus	36.02	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-3.47		Cheméo Relay (1.0)
logp	1.683		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method

tb	590.58	K	Cheméo Relay (1.0)
tc	901.27	K	Cheméo Relay (1.0)
tf	503.03	K	Cheméo Relay (1.0)
vc	0.542	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80137&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