2,4-Disulfamoyl-5-chloroaniline

Other names: 5-Chloro-2,4-disulfamylaniline
m-Chloroaniline-4,6-disulfonamide
1-Amino-3-chloro-4,6-benzenedisulfonamide
1,3-Benzenedisulfonamide, 4-amino-6-chloro-
m-Benzenedisulfonamide, 4-amino-6-chloro-
Chloraminophenamide
Chloroaminophenamide
Idorese
Salamid
Salmid
Su 5683
3-Chloro-4,6-disulfamoylaniline
4-Amino-6-chloro-m-benzenedisulfonamide
5-Chloro-2,4-disulfamoylaniline
4-Amino-6-chloro-1,3-benzenedisulfonamide
1,3-Disulfonamide, 4-amino-6-chlorobenzene-
4-amino-6-chlorobenzene-1,3-disulphonamide

Inchi: InChI=1S/C6H8ClN3O4S2/c7-3-1-4(8)6(16(10,13)14)2-5(3)15(9,11)12/h1-2H,8H2,(H2,9,

InchiKey: IHJCXVZDYSXXFT-UHFFFAOYSA-N

Formula: C6H8ClN3O4S2

SMILES: Nc1cc(Cl)c(S(N)(=O)=O)cc1S(N)(=O)=O

Mol. weight [g/mol]: 285.73

Physical Properties

Property code	Value	Unit	Source
hfus	46.71	kJ/mol	Joback Method
log10ws	-3.06		Cheméo Relay (1.0)
logp	-0.783		Crippen Method
mcvol	170.000	ml/mol	McGowan Method
tf	479.18	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	415.95	J/mol×K	728.88	Joback Method
cpg	424.72	J/mol×K	767.87	Joback Method
cpg	432.52	J/mol×K	806.86	Joback Method
cpg	439.32	J/mol×K	845.85	Joback Method
cpg	445.09	J/mol×K	884.84	Joback Method
cpg	449.80	J/mol×K	923.83	Joback Method
cpg	453.44	J/mol×K	962.82	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121302&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

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point