

N-Acetylsulfanilyl chloride

Other names:	p-Acetaminobenzenesulfonyl chloride p-Acetyl aminobenzene sulfonyl chloride 4-Acetamidobenzenesulfonyl chloride Benzenesulfonyl chloride, 4-(acetamino)- p-Acetamidobenzenesulfonyl chloride p-Acetamidophenylsulfonyl chloride p-Acetylamino benzenesulfochloride Acetanilide-p-sulfonyl chloride Acetylsulfanilyl chloride ASC Dagenan chloride N4-Acetylsulfanilyl chloride Sulfanilyl chloride, N-acetyl- 4-Acetamidophenylsulfonyl chloride 4'-(Chlorosulfonyl)acetanilide 4-Acetylamino-benzenesulfonyl chloride 4-Chlorosulfonylacetanilide NSC 127860 p-(Chlorosulfonyl)acetanilide N-acetylsulphanilyl chloride
Inchi:	InChI=1S/C8H8ClNO3S/c1-6(11)10-7-2-4-8(5-3-7)14(9,12)13/h2-5H,1H3,(H,10,11)
InchiKey:	GRDXCFKBQWDAJH-UHFFFAOYSA-N
Formula:	C8H8ClNO3S
SMILES:	CC(=O)Nc1ccc(S(=O)(=O)Cl)cc1
Mol. weight [g/mol]:	233.67
CAS:	121-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-400.74	kJ/mol	Joback Method
hf	-511.59	kJ/mol	Joback Method
hfus	32.40	kJ/mol	Joback Method
hvap	72.54	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.573		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method

tb	603.35	K	Joback Method
tc	822.48	K	Joback Method
tf	389.93	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.94	J/mol×K	603.35	Joback Method
cpg	346.01	J/mol×K	639.87	Joback Method
cpg	356.28	J/mol×K	676.39	Joback Method
cpg	365.76	J/mol×K	712.92	Joback Method
cpg	374.46	J/mol×K	749.44	Joback Method
cpg	382.40	J/mol×K	785.96	Joback Method
cpg	389.57	J/mol×K	822.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C121608&Units=SI

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

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