N-Acetylsulfanilyl chloride

Other names:	p-Acetaminobenzenesulfonyl chloride
	p-Acetyl aminobenzene sulfonyl chloride
	4-Acetamidobenzenesulfonyl chloride
	Benzenesulfonyl chloride, 4-(acetylamino)-
	p-Acetamidobenzenesulfonyl chloride
	p-Acetamidophenylsulfonyl chloride
	p-Acetylaminobenzenesulfochloride
	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	m3/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: 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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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