4-Acetylamino-benzenesulfonyl 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]:	233.68

Physical Properties

Property code	Value	Unit	Source
hfus	32.40	kJ/mol	Joback Method
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	1.572		Crippen Method
mcvol	151.700	ml/mol	McGowan Method
tb	591.06	K	Cheméo Relay (1.0)
tf	439.33	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121608&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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.