Acetanilide, 4-mercapto-

Other names:	Acetanilide, 4'-mercapto-
	p-Acetamidobenzenethiol
	p-Acetamidothiophenol
	4-(Acetylamino)benzenethiol
	4-Acetamidobenzenethiol
	4-Acetamidothiophenol
	4-Acetaminothiophenol
	4-Acetylaminothiophenol
	4'-Mercaptoacetanilide
	p-Acetaminothiophenol
	Acetanilide, 4-mercapto-
Inchi:	InChI=1S/C8H9NOS/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)
InchiKey:	AYEQJLOHMLYKAV-UHFFFAOYSA-N
Formula:	C8H9NOS
SMILES:	CC(=O)Nc1ccc(S)cc1
Mol. weight [g/mol]:	167.23

Physical Properties

Property code	Value	Unit	Source
hfus	20.87	kJ/mol	Joback Method
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	1.934		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
tb	577.96	K	Cheméo Relay (1.0)
tf	371.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.83	J/mol×K	581.00	Joback Method
cpg	289.49	J/mol×K	621.78	Joback Method
cpg	300.29	J/mol×K	662.57	Joback Method
cpg	310.27	J/mol×K	703.35	Joback Method

cpg	319.48	J/mol×K	744.14	Joback Method
cpg	327.94	J/mol×K	784.92	Joback Method
cpg	335.69	J/mol×K	825.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126814&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):	
Cheméo Relay (1.0, beta):	

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