

Acetamide, N-(4-mercaptophenyl)-

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
CAS:	1126-81-4

Physical Properties

Property code	Value	Unit	Source
gf	109.12	kJ/mol	Joback Method
hf	-4.02	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.934		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	581.00	K	Joback Method
tc	825.70	K	Joback Method
tf	357.91	K	Joback Method
vc	0.470	m3/kmol	Joback Method

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

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=C1126814&Units=SI
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
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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