

Acetamide, N-(«beta»-mercaptoethyl)-

Other names:	Acetamide, N-(2-mercaptoethyl)- Acetylcysteamine Cysteamine, N-acetyl- Ethanethiol, 2-(acetylamino)- N-(2-Mercaptoethyl)acetamide N-Acetyl cysteamin N-Acetylcysteamine N-Acetylmercaptoethylamine 2-Acetamidoethanethiol NSC 38835 N-(2-mercaptoethyl)acetamide (n-acetylcysteamine)
Inchi:	InChI=1S/C4H9NOS/c1-4(6)5-2-3-7/h7H,2-3H2,1H3,(H,5,6)
InchiKey:	AXFZADXWLMXITO-UHFFFAOYSA-N
Formula:	C4H9NOS
SMILES:	CC(=O)NCCS
Mol. weight [g/mol]:	119.19
CAS:	1190-73-4

Physical Properties

Property code	Value	Unit	Source
gf	-27.34	kJ/mol	Joback Method
hf	-146.52	kJ/mol	Joback Method
hfus	16.86	kJ/mol	Joback Method
hvap	44.42	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.052		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	457.82	K	Joback Method
tc	666.20	K	Joback Method
tf	273.89	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.17	J/mol×K	457.82	Joback Method
cpg	192.02	J/mol×K	492.55	Joback Method
cpg	200.43	J/mol×K	527.28	Joback Method
cpg	208.42	J/mol×K	562.01	Joback Method
cpg	215.99	J/mol×K	596.74	Joback Method
cpg	223.15	J/mol×K	631.47	Joback Method
cpg	229.92	J/mol×K	666.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1190734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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