Ethanethioic acid, S-[2-(acetylamino)ethyl] ester

Other names: Acetic acid, thio-, S-ester with N-(2-mercaptoethyl)acetamide
N,S-Diacetylcysteamine
S-(2-Acetamidoethyl) thiolacetate
S-Acetyl-N-acetylcysteamine
N,S-Diacetyl-«beta»-mercaptoethylamine
N,S-Diacetyl-2-mercaptoethylamine
Thioacetic acid S-2-acetamidoethyl ester
S-[2-(acetylamino)ethyl] ethanethioate
«beta»-Acetylaminoethylthiolacetate

Inchi: InChI=1S/C6H11NO2S/c1-5(8)7-3-4-10-6(2)9/h3-4H2,1-2H3,(H,7,8)

InchiKey: UZLRPNHVKXCOHS-UHFFFAOYSA-N

Formula: C6H11NO2S

SMILES: CC(=O)NCCSC(C)=O

Mol. weight [g/mol]: 161.22

CAS: 1420-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-135.69	kJ/mol	Joback Method
hf	-296.99	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.402		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	563.37	K	Joback Method
tc	774.56	K	Joback Method
tf	344.30	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	279.68	J/mol×K	563.37	Joback Method
cpg	290.10	J/mol×K	598.57	Joback Method
cpg	299.94	J/mol×K	633.77	Joback Method
cpg	309.23	J/mol×K	668.96	Joback Method
cpg	317.96	J/mol×K	704.16	Joback Method
cpg	326.15	J/mol×K	739.36	Joback Method
cpg	333.80	J/mol×K	774.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.70	K	2.00	NIST Webbook

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=C1420888&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume