

Acetamide, 2,2'-thiobis-

Other names:	2,2'-Thiodiacetamide 2,2'-Thiobisacetamide Thiodiacetamide
Inchi:	InChI=1S/C4H8N2O2S/c5-3(7)1-9-2-4(6)8/h1-2H2,(H2,5,7)(H2,6,8)
InchiKey:	KQNFZEVUCSXNTH-UHFFFAOYSA-N
Formula:	C4H8N2O2S
SMILES:	NC(=O)CSCC(N)=O
Mol. weight [g/mol]:	148.18
CAS:	14618-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-109.02	kJ/mol	Joback Method
hf	-241.60	kJ/mol	Joback Method
hfus	23.84	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	0.20		Crippen Method
logp	-1.310		Crippen Method
mcvol	106.670	ml/mol	McGowan Method
pc	5527.84	kPa	Joback Method
tb	612.50	K	Joback Method
tc	848.55	K	Joback Method
tf	435.62	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.49	J/molxK	612.50	Joback Method
cpg	254.54	J/molxK	651.84	Joback Method
cpg	262.03	J/molxK	691.18	Joback Method
cpg	268.98	J/molxK	730.53	Joback Method
cpg	275.39	J/molxK	769.87	Joback Method
cpg	281.26	J/molxK	809.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C14618656&Units=SI

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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