

Acetamide, N-(aminothioxomethyl)-

Other names:	Urea, 1-acetyl-2-thio- Acetothiourea Acetylthiourea N-Acetyl-2-thiourea N-Acetylthiocarbamide N-Acetylthiourea 1-Acetyl-2-thiourea 1-Acetylthiourea USAF EK-4890 Rcra waste number P002 Acetylthiocarbamide NSC 7597 acetyl-2-thiourea
Inchi:	InChI=1S/C3H6N2OS/c1-2(6)5-3(4)7/h1H3,(H3,4,5,6,7)
InchiKey:	IPCRBOOJBPE TMF-UHFFFAOYSA-N
Formula:	C3H6N2OS
SMILES:	CC(=O)NC(N)=S
Mol. weight [g/mol]:	118.16
CAS:	591-08-2

Physical Properties

Property code	Value	Unit	Source
gf	118.36	kJ/mol	Joback Method
hf	15.93	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	-0.634		Crippen Method
mcvol	86.710	ml/mol	McGowan Method
pc	6093.99	kPa	Joback Method
tb	514.65	K	Joback Method
tc	743.50	K	Joback Method
tf	343.69	K	Joback Method
vc	0.309	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.01	J/mol×K	514.65	Joback Method
cpg	179.73	J/mol×K	552.79	Joback Method
cpg	185.91	J/mol×K	590.93	Joback Method
cpg	191.60	J/mol×K	629.08	Joback Method
cpg	196.84	J/mol×K	667.22	Joback Method
cpg	201.68	J/mol×K	705.36	Joback Method
cpg	206.17	J/mol×K	743.50	Joback Method

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=C591082&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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