L-Methionine, N-acetyl-

Other names:	2-acetamido-4-methylsulfanylbutanoic acid
	Acetyl-L-methionine
	Acetylmethionin
	Acetylmethionine
	L-(N-Acetyl)methionine
	Methionamine
	Methionine, N-acetyl-, L-
	N-Acetyl-L-methionine
	N-Acetylmethionine
	Thiomedon
Inchi:	InChI=1S/C7H13NO3S/c1-5(9)8-6(7(10)11)3-4-12-2/h6H,3-4H2,1-2H3,(H,8,9)(H,10,11)/t
InchiKey:	XUYPXLNMDZIRQH-LURJTMIESA-N
Formula:	C7H13NO3S
SMILES:	CSCCC(NC(C)=O)C(=O)O
Mol. weight [g/mol]:	191.25
CAS:	65-82-7

Physical Properties

Property code	Value	Unit	Source
gf	-266.53	kJ/mol	Joback Method
hf	-475.14	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	74.21	kJ/mol	Joback Method
log10ws	0.03		Aqueous Solubility Prediction Method
logp	0.329		Crippen Method
mcvol	144.830	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	677.99	K	Joback Method
tc	876.76	K	Joback Method
tf	378.65	K	Aqueous Solubility Prediction Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.84	J/mol×K	677.99	Joback Method
cpg	381.38	J/mol×K	711.12	Joback Method
cpg	390.34	J/mol×K	744.25	Joback Method
cpg	398.73	J/mol×K	777.37	Joback Method
cpg	406.57	J/mol×K	810.50	Joback Method
cpg	413.86	J/mol×K	843.63	Joback Method
cpg	420.61	J/mol×K	876.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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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