2-Amino-4-(methylthio)butyric acid

Other names:	(S)-2-Amino-4-(methylthio)butanoic acid 2-Amino-4-methylthiobutanoic acid 2-Amino-4-methylthiobutanoic acid (S)- Acimethin Butanoic acid, 2-amino-4-(methylthio)-, (S)- Butyric acid, 2-amino-4-(methylthio)- Cymethion L(-)-Amino-«gamma»-methylthiobutyric acid L-(-)-Methionine L-2-Amino-4-(methylthio)butyric acid L-Homocysteine, S-methyl- L-methionine L-«alpha»-Amino-«gamma»-methylmercaptobutyric acid L-«gamma»-Methylthio-«alpha»-aminobutyric acid Liquimeth Met Methionine Methionine, L- NSC 22946 S-Methionine h-Met-oh «gamma»-Methylthio-«alpha»-aminobutyric acid
Inchi:	InChI=1S/C5H11NO2S/c1-9-3-2-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)
InchiKey:	FFEARJCKVFRZRR-SCSAIBSYSA-N
Formula:	C5H11NO2S
SMILES:	CSCCC(N)C(=O)O
Mol. weight [g/mol]:	149.22
CAS:	63-68-3

Physical Properties

Property code	Value	Unit	Source
hf	-428.97	kJ/mol	Cheméo Relay (1.0)
hfus	20.20	kJ/mol	Joback Method
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	0.18		Cheméo Relay (1.0)
logp	0.151		Crippen Method

mcvol	115.080	ml/mol	McGowan Method
tf	475.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.83	J/mol×K	600.72	Joback Method
cpg	283.51	J/mol×K	634.79	Joback Method
cpg	291.70	J/mol×K	668.86	Joback Method
cpg	299.43	J/mol×K	702.93	Joback Method
cpg	306.70	J/mol×K	737.00	Joback Method
cpg	313.51	J/mol×K	771.07	Joback Method
cpg	319.87	J/mol×K	805.14	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.71590e+01
Coeff. B	-1.50359e+04
Temperature range (K), min.	559.55
Temperature range (K), max.	688.22

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C59518

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tf:	Normal melting (fusion) point