

D-Methionine

Other names:	Methionine, D- R-Methionine D-Metionien d-2-Amino-4-(methylthio)butyric acid Methionine d-form D-(l)-methionine
Inchi:	InChI=1S/C5H11NO2S/c1-9-3-2-4(6)5(7)8/h4H,2-3,6H2,1H3,(H,7,8)/t4-/m0/s1
InchiKey:	FFEARJCKVFRZRR-BYPYZUCNSA-N
Formula:	C5H11NO2S
SMILES:	CSCCC(N)C(=O)O
Mol. weight [g/mol]:	149.21
CAS:	348-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-177.39	kJ/mol	Joback Method
hf	-340.96	kJ/mol	Joback Method
hfus	20.20	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.151		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	4684.89	kPa	Joback Method
tb	600.72	K	Joback Method
tc	805.14	K	Joback Method
tf	359.52	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.83	J/molxK	600.72	Joback Method
cpg	283.51	J/molxK	634.79	Joback Method
cpg	291.70	J/molxK	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
hsubt	125.10 ± 0.80	kJ/mol	455.00	NIST Webbook

Sources

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=C348674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hsubt:	Enthalpy of sublimation at a given temperature
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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