

# I-Methionine, N-(m-toluoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C14H19NO3S/c1-10-5-4-6-11(9-10)13(16)15-12(7-8-19-3)14(17)18-2/h4-6,9,11
<b>InchiKey:</b>	WWJYGVJTMIVDIA-UHFFFAOYSA-N
<b>Formula:</b>	C14H19NO3S
<b>SMILES:</b>	COC(=O)C(CCSC)NC(=O)c1cccc(C)c1
<b>Mol. weight [g/mol]:</b>	281.37

## Physical Properties

Property code	Value	Unit	Source
gf	-72.99	kJ/mol	Joback Method
hf	-374.55	kJ/mol	Joback Method
hfus	35.76	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.020		Crippen Method
mvol	219.700	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	800.05	K	Joback Method
tc	1024.98	K	Joback Method
tf	480.63	K	Joback Method
vc	0.825	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.54	J/mol×K	800.05	Joback Method
cpg	635.00	J/mol×K	837.54	Joback Method
cpg	647.34	J/mol×K	875.03	Joback Method
cpg	658.57	J/mol×K	912.51	Joback Method
cpg	668.71	J/mol×K	950.00	Joback Method
cpg	677.79	J/mol×K	987.49	Joback Method
cpg	685.83	J/mol×K	1024.98	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299641&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299641&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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