

# L-Methionine, N-(3-trifluoromethylbenzoyl)-, methyl ester

<b>Other names:</b>	L-Methione, N-(3-trifluoromethylbenzoyl)-, methyl ester
<b>Inchi:</b>	InChI=1S/C14H16F3NO3S/c1-21-13(20)11(6-7-22-2)18-12(19)9-4-3-5-10(8-9)14(15,16)1
<b>InchiKey:</b>	GIHUTHNRDKAYDT-UHFFFAOYSA-N
<b>Formula:</b>	C14H16F3NO3S
<b>SMILES:</b>	<chem>COC(=O)C(CCSC)NC(=O)c1cccc(C(F)(F)F)c1</chem>
<b>Mol. weight [g/mol]:</b>	335.34

## Physical Properties

Property code	Value	Unit	Source
gf	-654.58	kJ/mol	Joback Method
hf	-971.63	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.730		Crippen Method
mcvol	225.010	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	794.63	K	Joback Method
tc	1006.18	K	Joback Method
tf	484.82	K	Joback Method
vc	0.868	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.34	J/molxK	794.63	Joback Method
cpg	658.40	J/molxK	829.89	Joback Method
cpg	669.46	J/molxK	865.15	Joback Method
cpg	679.57	J/molxK	900.41	Joback Method
cpg	688.75	J/molxK	935.67	Joback Method
cpg	697.06	J/molxK	970.93	Joback Method
cpg	704.52	J/molxK	1006.18	Joback Method

# Sources

<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=U299701&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299701&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvp:</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>rlnol:</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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