

# L-Methionine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C13H14F3NO3S/c1-20-13(19)9(5-6-21-2)17-12(18)7-3-4-8(14)11(16)10(7)15/h
<b>InchiKey:</b>	XYKFYDOUYWEUTK-UHFFFAOYSA-N
<b>Formula:</b>	C13H14F3NO3S
<b>SMILES:</b>	COC(=O)C(CCSC)NC(=O)c1ccc(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	321.31

## Physical Properties

Property code	Value	Unit	Source
gf	-685.10	kJ/mol	Joback Method
hf	-965.18	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	75.11	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.128		Crippen Method
mcvol	210.920	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	784.94	K	Joback Method
tc	991.68	K	Joback Method
tf	496.17	K	Joback Method
vc	0.823	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.47	J/mol×K	784.94	Joback Method
cpg	598.86	J/mol×K	819.40	Joback Method
cpg	609.37	J/mol×K	853.85	Joback Method
cpg	618.99	J/mol×K	888.31	Joback Method
cpg	627.72	J/mol×K	922.77	Joback Method
cpg	635.58	J/mol×K	957.22	Joback Method
cpg	642.57	J/mol×K	991.68	Joback Method

# Sources

<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=U299632&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299632&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>

# 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>h vap:</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>r in pol:</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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