

# I-Methionine, n-heptafluorobutyryl-, pentyl ester

<b>Inchi:</b>	InChI=1S/C14H20F7NO3S/c1-3-4-5-7-25-10(23)9(6-8-26-2)22-11(24)12(15,16)13(17,18)
<b>InchiKey:</b>	SIRQYVCEKSOANO-UHFFFAOYSA-N
<b>Formula:</b>	C14H20F7NO3S
<b>SMILES:</b>	CCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	415.37

## Physical Properties

Property code	Value	Unit	Source
gf	-1530.92	kJ/mol	Joback Method
hf	-1998.63	kJ/mol	Joback Method
hfus	41.43	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.791		Crippen Method
mvol	255.850	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	753.59	K	Joback Method
tc	932.37	K	Joback Method
tf	453.08	K	Joback Method
vc	1.026	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.62	J/molxK	753.59	Joback Method
cpg	786.29	J/molxK	783.39	Joback Method
cpg	798.12	J/molxK	813.18	Joback Method
cpg	809.15	J/molxK	842.98	Joback Method
cpg	819.42	J/molxK	872.78	Joback Method
cpg	829.00	J/molxK	902.58	Joback Method
cpg	837.93	J/molxK	932.37	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=U320853&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320853&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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