

# L-Methionine, n-heptafluorobutyryl-, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C23H38F7NO3S/c1-3-4-5-6-7-8-9-10-11-12-13-14-16-34-19(32)18(15-17-35-2
<b>InchiKey:</b>	YQPKMJSNXAVJSX-UHFFFAOYSA-N
<b>Formula:</b>	C23H38F7NO3S
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	541.61

## Physical Properties

Property code	Value	Unit	Source
gf	-1455.14	kJ/mol	Joback Method
hf	-2184.39	kJ/mol	Joback Method
hfus	64.74	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.302		Crippen Method
mcvol	382.660	ml/mol	McGowan Method
pc	799.34	kPa	Joback Method
rinsol	2455.00		NIST Webbook
tb	959.51	K	Joback Method
tc	1183.43	K	Joback Method
tf	554.51	K	Joback Method
vc	1.530	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.60	J/molxK	959.51	Joback Method
cpg	1318.96	J/molxK	996.83	Joback Method
cpg	1335.09	J/molxK	1034.15	Joback Method
cpg	1350.11	J/molxK	1071.47	Joback Method
cpg	1364.16	J/molxK	1108.79	Joback Method
cpg	1377.38	J/molxK	1146.11	Joback Method
cpg	1389.88	J/molxK	1183.43	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=U320860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320860&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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