

# L-Methionine, n-pentafluoropropionyl-, dodecyl ester

<b>Inchi:</b>	InChI=1S/C20H34F5NO3S/c1-3-4-5-6-7-8-9-10-11-12-14-29-17(27)16(13-15-30-2)26-18
<b>InchiKey:</b>	MPJHLDRVTBZNEK-UHFFFAOYSA-N
<b>Formula:</b>	C20H34F5NO3S
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(CCSC)NC(=O)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	463.55

## Physical Properties

Property code	Value	Unit	Source
gf	-1093.62	kJ/mol	Joback Method
hf	-1721.50	kJ/mol	Joback Method
hfus	58.22	kJ/mol	Joback Method
hvap	82.20	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.886		Crippen Method
mvol	336.850	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2378.00		NIST Webbook
tb	895.56	K	Joback Method
tc	1096.58	K	Joback Method
tf	517.10	K	Joback Method
vc	1.337	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.23	J/molxK	895.56	Joback Method
cpg	1120.05	J/molxK	929.06	Joback Method
cpg	1134.77	J/molxK	962.57	Joback Method
cpg	1148.45	J/molxK	996.07	Joback Method
cpg	1161.16	J/molxK	1029.57	Joback Method
cpg	1172.97	J/molxK	1063.07	Joback Method
cpg	1183.95	J/molxK	1096.58	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=U320920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320920&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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