

# Aspartic acid-phenylalanine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C19H23F3N2O6/c1-23(14(17(27)30-4)10-12-8-6-5-7-9-12)16(26)13(11-15(25))  
InChIKey: LCJUOZRBMKERRC-UHFFFAOYSA-N

Formula: C19H23F3N2O6

SMILES: COC(=O)CC(C(=O)N(C)C(Cc1ccccc1)C(=O)OC)N(C)C(=O)C(F)(F)F

Mol. weight [g/mol]: 432.39

## Physical Properties

Property code	Value	Unit	Source
gf	-869.08	kJ/mol	Joback Method
hf	-1386.30	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.181		Crippen Method
mcvol	298.100	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	939.70	K	Joback Method
tc	1152.81	K	Joback Method
tf	613.62	K	Joback Method
vc	1.119	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.82	J/molxK	939.70	Joback Method
cpg	966.46	J/molxK	975.22	Joback Method
cpg	976.99	J/molxK	1010.74	Joback Method
cpg	986.46	J/molxK	1046.25	Joback Method
cpg	994.95	J/molxK	1081.77	Joback Method
cpg	1002.52	J/molxK	1117.29	Joback Method
cpg	1009.25	J/molxK	1152.81	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=R248738&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R248738&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>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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