

# Phe,TFE-PFP

<b>Other names:</b>	Phenylalanine, TFE-PFP
<b>Inchi:</b>	InChI=1S/C14H11F8NO3/c15-12(16,17)7-26-10(24)9(6-8-4-2-1-3-5-8)23-11(25)13(18,19
<b>InchiKey:</b>	POECKMJIDGHMCD-UHFFFAOYSA-N
<b>Formula:</b>	C14H11F8NO3
<b>SMILES:</b>	O=C(OCC(F)(F)F)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	393.23

## Physical Properties

Property code	Value	Unit	Source
gf	-1646.44	kJ/mol	Joback Method
hf	-2000.08	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	60.56	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.017		Crippen Method
mcvol	217.510	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
tb	710.76	K	Joback Method
tc	892.13	K	Joback Method
tf	445.69	K	Joback Method
vc	0.881	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.37	J/molxK	710.76	Joback Method
cpg	650.65	J/molxK	740.99	Joback Method
cpg	661.06	J/molxK	771.22	Joback Method
cpg	670.66	J/molxK	801.45	Joback Method
cpg	679.51	J/molxK	831.67	Joback Method
cpg	687.67	J/molxK	861.90	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=R57171&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R57171&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>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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