

Tyr, HFIP-PFP

Other names:	Tyrosine, HFIP-PFP
Inchi:	InChI=1S/C18H9F16NO5/c19-13(20,17(29,30)31)11(37)35-8(9(36)40-10(15(23,24)25)16
InchiKey:	YJHBADMGEIKSNX-UHFFFAOYSA-N
Formula:	C18H9F16NO5
SMILES:	O=C(OC(C(F)(F)F)C(F)(F)F)C(Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	623.24

Physical Properties

Property code	Value	Unit	Source
gf	-3408.71	kJ/mol	Joback Method
hf	-3939.32	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.051		Crippen Method
mcvol	295.470	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
tb	867.58	K	Joback Method
tc	1063.01	K	Joback Method
tf	572.43	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.78	J/molxK	867.58	Joback Method
cpg	966.89	J/molxK	900.15	Joback Method
cpg	975.20	J/molxK	932.72	Joback Method
cpg	982.83	J/molxK	965.29	Joback Method
cpg	989.91	J/molxK	997.87	Joback Method
cpg	996.57	J/molxK	1030.44	Joback Method
cpg	1002.92	J/molxK	1063.01	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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