

Tyr, TFE-PFP

Other names:	Tyrosine, TFE-PFP
Inchi:	InChI=1S/C17H10F13NO5/c18-13(19,20)6-35-10(32)9(31-11(33)14(21,22)16(25,26)27)5
InchiKey:	VETSZNAHNSVCCT-UHFFFAOYSA-N
Formula:	C17H10F13NO5
SMILES:	O=C(OCC(F)(F)F)C(Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1)N=C(O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	555.24

Physical Properties

Property code	Value	Unit	Source
hf	-3337.01	kJ/mol	Joback Method
hvap	77.27	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.960		Crippen Method
mcvol	276.070	ml/mol	McGowan Method
pc	1163.25	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	915.26	K	Joback Method
tc	1121.92	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R57199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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

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