

Lysine-tyrosine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C24H31F6N3O6/c1-31(21(36)23(25,26)27)13-7-6-8-17(33(3)22(37)24(28,29)3
InChIKey: YELVAZIGNWFQKJ-UHFFFAOYSA-N
Formula: C24H31F6N3O6
SMILES: COC(=O)C(Cc1ccc(OC)cc1)N(C)C(=O)C(CCCCN(C)C(=O)C(F)(F)F)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 571.51

Physical Properties

Property code	Value	Unit	Source
gf	-1307.42	kJ/mol	Joback Method
hf	-2030.52	kJ/mol	Joback Method
hfus	66.01	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	2.818		Crippen Method
mcvol	383.840	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2888.00		NIST Webbook
tb	1066.10	K	Joback Method
tc	1319.17	K	Joback Method
tf	719.15	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.72	J/molxK	1066.10	Joback Method
cpg	1327.28	J/molxK	1108.28	Joback Method
cpg	1339.61	J/molxK	1150.46	Joback Method
cpg	1350.90	J/molxK	1192.64	Joback Method
cpg	1361.33	J/molxK	1234.82	Joback Method
cpg	1371.09	J/molxK	1276.99	Joback Method
cpg	1380.37	J/molxK	1319.17	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248763&Units=SI

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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