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

Inchi: InChI=1S/C29H40F6N4O8/c1-36(26(43)28(30,31)32)15-9-8-10-20(37(2)24(41)22(17-45-

InchiKey: XUMUKDSKWUEAAH-UHFFFAOYSA-N

Formula: C29H40F6N4O8

SMILES: COCC(C(=O)N(C)C(CCCCN(C)C(=O)C(F)(F)F)C(=O)N(C)C(Cc1ccc(OC)cc1)C(=O)OC)N

Mol. weight [g/mol]: 686.64

Physical Properties

Property code	Value	Unit	Source
gf	-1390.90	kJ/mol	Joback Method
hf	-2316.27	kJ/mol	Joback Method
hfus	81.24	kJ/mol	Joback Method
hvap	123.56	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.291		Crippen Method
mcvol	471.710	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	3461.00		NIST Webbook
rinpol	3380.00		NIST Webbook
rinpol	3380.00		NIST Webbook
tb	1268.79	K	Joback Method
tc	1659.13	K	Joback Method
tf	865.13	K	Joback Method
vc	1.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.88	J/mol×K	1268.79	Joback Method
cpg	1702.65	J/mol×K	1333.85	Joback Method
cpg	1715.81	J/mol×K	1398.90	Joback Method
cpg	1728.08	J/mol×K	1463.96	Joback Method
cpg	1740.23	J/mol×K	1529.02	Joback Method
cpg	1752.99	J/mol×K	1594.08	Joback Method
cpg	1767.11	J/mol×K	1659.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume