

Glycine-threonine-phenylalanine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C22H30F3N3O6/c1-14(33-5)18(28(4)17(29)13-26(2)21(32)22(23,24)25)19(30)
InChIKey: YNJPSXZBYFXIQK-UHFFFAOYSA-N
Formula: C22H30F3N3O6
SMILES: COC(=O)C(Cc1ccccc1)N(C)C(=O)C(C(C)OC)N(C)C(=O)CN(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 489.49

Physical Properties

Property code	Value	Unit	Source
gf	-735.48	kJ/mol	Joback Method
hf	-1385.97	kJ/mol	Joback Method
hfus	55.87	kJ/mol	Joback Method
hvap	99.86	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.112		Crippen Method
mcvol	350.350	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	1020.34	K	Joback Method
tc	1249.84	K	Joback Method
tf	664.90	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.48	J/mol×K	1020.34	Joback Method
cpg	1187.03	J/mol×K	1058.59	Joback Method
cpg	1198.33	J/mol×K	1096.84	Joback Method
cpg	1208.48	J/mol×K	1135.09	Joback Method
cpg	1217.60	J/mol×K	1173.34	Joback Method
cpg	1225.80	J/mol×K	1211.59	Joback Method
cpg	1233.18	J/mol×K	1249.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248743&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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