Methionine-asparagine-threonine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

InChI: InChI=1S/C21H34F3N3O8S/c1-12(33-5)16(19(31)35-7)27(4)18(30)14(11-15(28)34-6)25(
InChIKey: FWCOJIVFRVTKJP-UHFFFAOYSA-N
Formula: C21H34F3N3O8S
SMILES: COC(=O)CC(C(=O)N(C)C(C(=O)OC)C(C)OC)N(C)C(=O)C(CCSC)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 545.57

Physical Properties

Property code	Value	Unit	Source
gf	-1059.55	kJ/mol	Joback Method
hf	-1810.07	kJ/mol	Joback Method
hfus	62.63	kJ/mol	Joback Method
hvap	110.95	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	0.554		Crippen Method
mcvol	383.810	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	2959.00		NIST Webbook
tb	1115.41	K	Joback Method
tc	1381.03	K	Joback Method
tf	718.77	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1304.08	J/mol×K	1115.41	Joback Method
cpg	1313.58	J/mol×K	1159.68	Joback Method
cpg	1321.03	J/mol×K	1203.95	Joback Method
cpg	1326.51	J/mol×K	1248.22	Joback Method
cpg	1330.14	J/mol×K	1292.49	Joback Method
cpg	1332.02	J/mol×K	1336.76	Joback Method
cpg	1332.26	J/mol×K	1381.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248778&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