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

Inchi: InChI=1S/C14H23F3N2O6/c1-8(24-5)10(19(3)13(22)14(15,16)17)11(20)18(2)9(7-23-4)12
InchiKey: NHBCWZCXGIHONC-UHFFFAOYSA-N
Formula: C14H23F3N2O6
SMILES: COCC(C(=O)OC)N(C)C(=O)C(C(C)OC)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 372.34

Physical Properties

Property code	Value	Unit	Source
gf	-1002.11	kJ/mol	Joback Method
hf	-1544.55	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	73.40	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.057		Crippen Method
mcvol	255.710	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	766.73	K	Joback Method
tc	948.44	K	Joback Method
tf	488.15	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.05	J/mol×K	766.73	Joback Method
cpg	793.97	J/mol×K	797.01	Joback Method
cpg	806.98	J/mol×K	827.30	Joback Method
cpg	819.08	J/mol×K	857.58	Joback Method
cpg	830.30	J/mol×K	887.87	Joback Method
cpg	840.66	J/mol×K	918.15	Joback Method
cpg	850.18	J/mol×K	948.44	Joback Method

Sources

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=R248798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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