Valine-glutamine, N(«alpha»,«epsilon»)-trifluoroacetyl-N-O-permeth derivative

Inchi: InChI=1S/C18H25F6N3O6/c1-9(2)12(27(5)16(32)18(22,23)24)13(29)25(3)10(14(30)33-6
InchiKey: OPUPPVHWLAMWRZ-UHFFFAOYSA-N
Formula: C18H25F6N3O6
SMILES: COC(=O)C(CCC(=O)N(C)C(=O)C(F)(F)F)N(C)C(=O)C(C(C)C)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 493.40

Physical Properties

Property code	Value	Unit	Source
gf	-1487.08	kJ/mol	Joback Method
hf	-2117.38	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	89.27	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.359		Crippen Method
mcvol	318.760	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	928.17	K	Joback Method
tc	1137.33	K	Joback Method
tf	625.29	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.94	J/mol×K	928.17	Joback Method
cpg	1060.45	J/mol×K	963.03	Joback Method
cpg	1071.95	J/mol×K	997.89	Joback Method
cpg	1082.56	J/mol×K	1032.75	Joback Method
cpg	1092.38	J/mol×K	1067.61	Joback Method
cpg	1101.49	J/mol×K	1102.47	Joback Method
cpg	1110.00	J/mol×K	1137.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248827&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

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