N-«alpha»-Methyl lysine, butyl ester, TFA

Inchi: InChI=1S/C15H22F6N2O4/c1-3-4-9-27-11(24)10(23(2)13(26)15(19,20)21)7-5-6-8-22-12(
InchiKey: DBVNRNMBQDPRTG-UHFFFAOYSA-N
Formula: C15H22F6N2O4
SMILES: CCCCOC(=O)C(CCCCNC(=O)C(F)(F)F)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 408.34

Physical Properties

Property code	Value	Unit	Source
gf	-1381.79	kJ/mol	Joback Method
hf	-1901.33	kJ/mol	Joback Method
hfus	48.84	kJ/mol	Joback Method
hvap	72.23	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.568		Crippen Method
mcvol	263.370	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook
tb	777.96	K	Joback Method
tc	955.18	K	Joback Method
tf	509.34	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.70	J/mol×K	777.96	Joback Method
cpg	832.77	J/mol×K	807.50	Joback Method
cpg	845.00	J/mol×K	837.03	Joback Method
cpg	856.43	J/mol×K	866.57	Joback Method
cpg	867.13	J/mol×K	896.11	Joback Method
cpg	877.14	J/mol×K	925.64	Joback Method
cpg	886.49	J/mol×K	955.18	Joback Method

Sources

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=R32030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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