lysine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C13H18F6N2O4/c1-7(2)25-9(22)8(21-11(24)13(17,18)19)5-3-4-6-20-10(23)12(
InchiKey: ROKQLTBITCEWNS-UHFFFAOYSA-N
Formula: C13H18F6N2O4
SMILES: CC(C)OC(=O)C(CCCCNC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 380.28

Physical Properties

Property code	Value	Unit	Source
gf	-1422.46	kJ/mol	Joback Method
hf	-1879.39	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	71.78	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	1.834		Crippen Method
mcvol	235.190	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook
tb	769.49	K	Joback Method
tc	948.80	K	Joback Method
tf	491.99	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.14	J/mol×K	769.49	Joback Method
cpg	735.80	J/mol×K	799.37	Joback Method
cpg	746.68	J/mol×K	829.26	Joback Method
cpg	756.82	J/mol×K	859.14	Joback Method
cpg	766.24	J/mol×K	889.03	Joback Method
cpg	775.01	J/mol×K	918.91	Joback Method
cpg	783.16	J/mol×K	948.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R267937&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