ornithine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C12H16F6N2O4/c1-6(2)24-8(21)7(20-10(23)12(16,17)18)4-3-5-19-9(22)11(13,
InchiKey: ISCJAKJOJMTBMT-UHFFFAOYSA-N
Formula: C12H16F6N2O4
SMILES: CC(C)OC(=O)C(CCCNC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 366.26

Physical Properties

Property code	Value	Unit	Source
gf	-1430.88	kJ/mol	Joback Method
hf	-1858.75	kJ/mol	Joback Method
hfus	39.62	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	1.444		Crippen Method
mcvol	221.100	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1603.00		NIST Webbook
tb	746.61	K	Joback Method
tc	924.27	K	Joback Method
tf	480.72	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.00	J/mol×K	746.61	Joback Method
cpg	681.21	J/mol×K	776.22	Joback Method
cpg	691.67	J/mol×K	805.83	Joback Method
cpg	701.41	J/mol×K	835.44	Joback Method
cpg	710.47	J/mol×K	865.05	Joback Method
cpg	718.88	J/mol×K	894.66	Joback Method
cpg	726.70	J/mol×K	924.27	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=R267957&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