L-Ornithine, N2,N5-bis(trifluoroacetyl)-, butyl ester

Other names: Ornitine, butyl ester, N2,N5-bis-TFA
Ornitine, butyl ester, TFA
Inchi: InChI=1S/C13H18F6N2O4/c1-2-3-7-25-9(22)8(21-11(24)13(17,18)19)5-4-6-20-10(23)12(
InchiKey: LMGYQYJQQMTKTR-MRVPVSSYSA-N
Formula: C13H18F6N2O4
SMILES: CCCCOC(=O)C(CCCNC(=O)C(F)(F)F)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 380.28
CAS: 2804-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-1420.02	kJ/mol	Joback Method
hf	-1874.11	kJ/mol	Joback Method
hfus	45.74	kJ/mol	Joback Method
hvap	72.17	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	1.836		Crippen Method
mcvol	235.190	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	769.93	K	Joback Method
tc	948.10	K	Joback Method
tf	506.99	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.56	J/mol×K	769.93	Joback Method
cpg	735.15	J/mol×K	799.63	Joback Method
cpg	745.96	J/mol×K	829.32	Joback Method
cpg	756.05	J/mol×K	859.02	Joback Method
cpg	765.45	J/mol×K	888.71	Joback Method

cpg	774.20	J/mol×K	918.41	Joback Method
cpg	782.34	J/mol×K	948.10	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=C2804684&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