D-Alanine, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, ethyl ester

Inchi: InChI=1S/C13H14F3NO4/c1-4-21-13(19)6(2)17-12(18)7-5-8(14)10(16)11(20-3)9(7)15/h5
InchiKey: AVEFJQGYAPMVDP-UHFFFAOYSA-N
Formula: C13H14F3NO4
SMILES: CCOC(=O)C(C)NC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 305.25

Physical Properties

Property code	Value	Unit	Source
gf	-832.85	kJ/mol	Joback Method
hf	-1150.74	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	1.794		Crippen Method
mcvol	200.440	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	743.56	K	Joback Method
tc	937.11	K	Joback Method
tf	496.52	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.54	J/mol×K	743.56	Joback Method
cpg	572.31	J/mol×K	775.82	Joback Method
cpg	583.33	J/mol×K	808.08	Joback Method
cpg	593.60	J/mol×K	840.34	Joback Method
cpg	603.09	J/mol×K	872.60	Joback Method
cpg	611.82	J/mol×K	904.85	Joback Method
cpg	619.77	J/mol×K	937.11	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=U348449&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