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

Inchi: InChI=1S/C14H16F3NO4/c1-4-5-22-14(20)7(2)18-13(19)8-6-9(15)11(17)12(21-3)10(8)16

InchiKey: HQNVNSKHICGIDT-UHFFFAOYSA-N

Formula: C14H16F3NO4

SMILES: CCCOC(=O)C(C)NC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 319.28

Physical Properties

Property code	Value	Unit	Source
gf	-824.43	kJ/mol	Joback Method
hf	-1171.38	kJ/mol	Joback Method
hfus	40.89	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.184		Crippen Method
mcvol	214.530	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1986.00		NIST Webbook
tb	766.44	K	Joback Method
tc	959.40	K	Joback Method
tf	507.79	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.27	J/mol×K	766.44	Joback Method
cpg	626.50	J/mol×K	798.60	Joback Method
cpg	637.92	J/mol×K	830.76	Joback Method
cpg	648.53	J/mol×K	862.92	Joback Method
cpg	658.33	J/mol×K	895.08	Joback Method
cpg	667.31	J/mol×K	927.24	Joback Method
cpg	675.47	J/mol×K	959.40	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=U348450&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