D-Alanine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, tridecyl ester

Inchi: InChI=1S/C24H35F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-17-32-23(31)18(2)29-22(30)19-1

InchiKey: QLSUXRKNXJLNRH-UHFFFAOYSA-N

Formula: C24H35F4NO3

SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 461.53

Physical Properties

Property code	Value	Unit	Source
gf	-807.94	kJ/mol	Joback Method
hf	-1427.48	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	90.00	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.817		Crippen Method
mcvol	351.330	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
rinpol	2753.00		NIST Webbook
tb	958.90	K	Joback Method
tc	1175.24	K	Joback Method
tf	576.23	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.25	J/mol×K	958.90	Joback Method
cpg	1194.46	J/mol×K	994.96	Joback Method
cpg	1209.41	J/mol×K	1031.01	Joback Method
cpg	1223.21	J/mol×K	1067.07	Joback Method
cpg	1235.91	J/mol×K	1103.13	Joback Method
cpg	1247.60	J/mol×K	1139.18	Joback Method
cpg	1258.37	J/mol×K	1175.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348424&Units=SI

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