D-alanine, n-(3-fluoro-5-trifluoromethylbenzoyl)-, tridecyl ester

Inchi: InChI=1S/C24H35F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-32-23(31)18(2)29-22(30)19-1

InchiKey: ZTEXQXRPDVHXAN-UHFFFAOYSA-N

Formula: C24H35F4NO3

SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 461.54

Physical Properties

Property code	Value	Unit	Source
hfus	62.05	kJ/mol	Joback Method
logp	6.817		Crippen Method
mcvol	351.330	ml/mol	McGowan Method
rinpol	2632.00		NIST Webbook

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U347812&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices