D-Alanine, N-(2-fluoro-6-trifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C22H31F4NO3/c1-3-4-5-6-7-8-9-10-11-15-30-21(29)16(2)27-20(28)19-17(22(2
InchiKey: BDPLHFAKLHIFJS-UHFFFAOYSA-N
Formula: C22H31F4NO3
SMILES: CCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 433.48

Physical Properties

Property code	Value	Unit	Source
gf	-824.78	kJ/mol	Joback Method
hf	-1386.20	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.037		Crippen Method
mcvol	323.150	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2612.00		NIST Webbook
tb	913.14	K	Joback Method
tc	1118.03	K	Joback Method
tf	553.69	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.69	J/mol×K	913.14	Joback Method
cpg	1071.99	J/mol×K	947.29	Joback Method
cpg	1086.17	J/mol×K	981.44	Joback Method
cpg	1099.31	J/mol×K	1015.58	Joback Method
cpg	1111.44	J/mol×K	1049.73	Joback Method
cpg	1122.65	J/mol×K	1083.88	Joback Method
cpg	1132.99	J/mol×K	1118.03	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=U348377&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

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