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

Inchi: InChI=1S/C25H37F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-33-24(32)19(2)30-23(31)2
InchiKey: HQOINDBVUBFUOB-UHFFFAOYSA-N
Formula: C25H37F4NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 475.56

Physical Properties

Property code	Value	Unit	Source
gf	-799.52	kJ/mol	Joback Method
hf	-1448.12	kJ/mol	Joback Method
hfus	64.64	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	7.207		Crippen Method
mcvol	365.420	ml/mol	McGowan Method
pc	892.13	kPa	Joback Method
rinpol	2927.00		NIST Webbook
tb	981.78	K	Joback Method
tc	1205.47	K	Joback Method
tf	587.50	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.87	J/mol×K	981.78	Joback Method
cpg	1256.59	J/mol×K	1019.06	Joback Method
cpg	1271.99	J/mol×K	1056.34	Joback Method
cpg	1286.15	J/mol×K	1093.63	Joback Method
cpg	1299.17	J/mol×K	1130.91	Joback Method
cpg	1311.13	J/mol×K	1168.19	Joback Method
cpg	1322.14	J/mol×K	1205.47	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=U348380&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