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

Inchi: InChI=1S/C31H49F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-39-30(
InchiKey: QZVPWDCFCFXWSP-UHFFFAOYSA-N
Formula: C31H49F4NO3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 559.72

Physical Properties

Property code	Value	Unit	Source
gf	-749.00	kJ/mol	Joback Method
hf	-1571.96	kJ/mol	Joback Method
hfus	80.18	kJ/mol	Joback Method
hvap	105.59	kJ/mol	Joback Method
log10ws	-11.43		Crippen Method
logp	9.548		Crippen Method
mcvol	449.960	ml/mol	McGowan Method
pc	649.44	kPa	Joback Method
rinpol	3536.00		NIST Webbook
rinpol	3536.00		NIST Webbook
tb	1119.06	K	Joback Method
tc	1415.58	K	Joback Method
tf	655.12	K	Joback Method
vc	1.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.87	J/mol×K	1119.06	Joback Method
cpg	1640.06	J/mol×K	1168.48	Joback Method
cpg	1659.20	J/mol×K	1217.90	Joback Method
cpg	1676.53	J/mol×K	1267.32	Joback Method
cpg	1692.34	J/mol×K	1316.74	Joback Method
cpg	1706.88	J/mol×K	1366.16	Joback Method
cpg	1720.42	J/mol×K	1415.58	Joback Method

Sources

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=U348386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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