D-Alanine, N-(3-fluoro-4-trifluoromethylbenzoyl)-, nonadecyl ester

Inchi: InChI=1S/C30H47F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-38-29(37)
InchiKey: KEZHMVPBKFHJET-UHFFFAOYSA-N
Formula: C30H47F4NO3
SMILES: CCCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 545.69

Physical Properties

Property code	Value	Unit	Source
gf	-757.42	kJ/mol	Joback Method
hf	-1551.32	kJ/mol	Joback Method
hfus	77.59	kJ/mol	Joback Method
hvap	103.36	kJ/mol	Joback Method
log10ws	-11.02		Crippen Method
logp	9.158		Crippen Method
mcvol	435.870	ml/mol	McGowan Method
pc	682.43	kPa	Joback Method
rinpol	3335.00		NIST Webbook
rinpol	3335.00		NIST Webbook
tb	1096.18	K	Joback Method
tc	1376.59	K	Joback Method
tf	643.85	K	Joback Method
vc	1.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.75	J/mol×K	1096.18	Joback Method
cpg	1575.00	J/mol×K	1142.92	Joback Method
cpg	1593.34	J/mol×K	1189.65	Joback Method
cpg	1610.00	J/mol×K	1236.39	Joback Method
cpg	1625.18	J/mol×K	1283.12	Joback Method
cpg	1639.11	J/mol×K	1329.86	Joback Method
cpg	1651.99	J/mol×K	1376.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347795&Units=SI
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

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