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

Inchi: InChI=1S/C28H43F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-36-27(35)22(2)3
Inchikey: OTEJDALKQDUQRB-UHFFFAOYSA-N
Formula: C28H43F4NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 517.64

Physical Properties

Property code	Value	Unit	Source
gf	-774.26	kJ/mol	Joback Method
hf	-1510.04	kJ/mol	Joback Method
hfus	72.41	kJ/mol	Joback Method
hvap	98.91	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.377		Crippen Method
mcvol	407.690	ml/mol	McGowan Method
pc	756.40	kPa	Joback Method
rinpol	3222.00		NIST Webbook
rinpol	3222.00		NIST Webbook
tb	1050.42	K	Joback Method
tc	1303.74	K	Joback Method
tf	621.31	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.57	J/mol×K	1050.42	Joback Method
cpg	1446.20	J/mol×K	1092.64	Joback Method
cpg	1463.18	J/mol×K	1134.86	Joback Method
cpg	1478.69	J/mol×K	1177.08	Joback Method
cpg	1492.85	J/mol×K	1219.30	Joback Method
cpg	1505.83	J/mol×K	1261.52	Joback Method
cpg	1517.76	J/mol×K	1303.74	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=U348383&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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