D-Alanine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, octadecyl ester

Inchi: InChI=1S/C29H45F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-37-28(36)23(
InchiKey: WBFUZMLEGKGRQK-UHFFFAOYSA-N
Formula: C29H45F4NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 531.67

Physical Properties

Property code	Value	Unit	Source
gf	-765.84	kJ/mol	Joback Method
hf	-1530.68	kJ/mol	Joback Method
hfus	75.00	kJ/mol	Joback Method
hvap	101.13	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	8.768		Crippen Method
mcvol	421.780	ml/mol	McGowan Method
pc	717.99	kPa	Joback Method
rinpol	3264.00		NIST Webbook
rinpol	3264.00		NIST Webbook
tb	1073.30	K	Joback Method
tc	1339.36	K	Joback Method
tf	632.58	K	Joback Method
vc	1.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.98	J/mol×K	1073.30	Joback Method
cpg	1510.37	J/mol×K	1117.64	Joback Method
cpg	1528.00	J/mol×K	1161.99	Joback Method
cpg	1544.05	J/mol×K	1206.33	Joback Method
cpg	1558.69	J/mol×K	1250.67	Joback Method
cpg	1572.10	J/mol×K	1295.01	Joback Method
cpg	1584.47	J/mol×K	1339.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348429&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

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