D-Alanine, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C27H42F3NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-35-27(33)20(2)31-
InchiKey: GCJWMYNKRPAOSG-UHFFFAOYSA-N
Formula: C27H42F3NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 501.62

Physical Properties

Property code	Value	Unit	Source
gf	-714.97	kJ/mol	Joback Method
hf	-1439.70	kJ/mol	Joback Method
hfus	74.56	kJ/mol	Joback Method
hvap	102.53	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	7.255		Crippen Method
mcvol	397.700	ml/mol	McGowan Method
pc	788.60	kPa	Joback Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook
tb	1063.88	K	Joback Method
tc	1322.73	K	Joback Method
tf	654.30	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.18	J/mol×K	1063.88	Joback Method
cpg	1400.84	J/mol×K	1107.02	Joback Method
cpg	1415.26	J/mol×K	1150.16	Joback Method
cpg	1427.50	J/mol×K	1193.30	Joback Method
cpg	1437.64	J/mol×K	1236.45	Joback Method
cpg	1445.74	J/mol×K	1279.59	Joback Method
cpg	1451.86	J/mol×K	1322.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348452&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

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