D-Alanine, N-(3-fluoro-5-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C27H41F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-35-26(34)21(2)32-2
InchiKey: VAXJSVMSXGLRGY-UHFFFAOYSA-N
Formula: C27H41F4NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 503.61

Physical Properties

Property code	Value	Unit	Source
gf	-782.68	kJ/mol	Joback Method
hf	-1489.40	kJ/mol	Joback Method
hfus	69.82	kJ/mol	Joback Method
hvap	96.68	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	7.987		Crippen Method
mcvol	393.600	ml/mol	McGowan Method
pc	797.98	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	1027.54	K	Joback Method
tc	1269.63	K	Joback Method
tf	610.04	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.57	J/mol×K	1027.54	Joback Method
cpg	1382.49	J/mol×K	1067.89	Joback Method
cpg	1398.90	J/mol×K	1108.24	Joback Method
cpg	1413.91	J/mol×K	1148.58	Joback Method
cpg	1427.65	J/mol×K	1188.93	Joback Method
cpg	1440.25	J/mol×K	1229.28	Joback Method
cpg	1451.83	J/mol×K	1269.63	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=U347815&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