D-Alanine, N-(2,5-ditrifluoromethylbenzoyl)-, octadecyl ester

Inchi: InChI=1S/C30H45F6NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-40-28(39)23(
InchiKey: QJQYTYDFIVCKQX-UHFFFAOYSA-N
Formula: C30H45F6NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 581.67

Physical Properties

Property code	Value	Unit	Source
gf	-1144.20	kJ/mol	Joback Method
hf	-1952.29	kJ/mol	Joback Method
hfus	76.33	kJ/mol	Joback Method
hvap	100.43	kJ/mol	Joback Method
log10ws	-11.37		Crippen Method
logp	9.647		Crippen Method
mcvol	439.410	ml/mol	McGowan Method
pc	657.80	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	1091.49	K	Joback Method
tc	1375.82	K	Joback Method
tf	647.45	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1567.69	J/mol×K	1091.49	Joback Method
cpg	1588.56	J/mol×K	1138.88	Joback Method
cpg	1607.82	J/mol×K	1186.27	Joback Method
cpg	1625.72	J/mol×K	1233.66	Joback Method
cpg	1642.57	J/mol×K	1281.05	Joback Method
cpg	1658.62	J/mol×K	1328.43	Joback Method
cpg	1674.17	J/mol×K	1375.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347807&Units=SI

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