D-Alanine, N-(2,6-difluoro-3-methylbenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C28H45F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-34-28(33)23(3)
InchiKey: OQNRAAXJLURWQU-UHFFFAOYSA-N
Formula: C28H45F2NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 481.66

Physical Properties

Property code	Value	Unit	Source
gf	-397.11	kJ/mol	Joback Method
hf	-1120.54	kJ/mol	Joback Method
hfus	73.27	kJ/mol	Joback Method
hvap	102.50	kJ/mol	Joback Method
log10ws	-9.88		Crippen Method
logp	7.806		Crippen Method
mcvol	404.150	ml/mol	McGowan Method
pc	780.25	kPa	Joback Method
rinpol	3403.00		NIST Webbook
tb	1060.09	K	Joback Method
tc	1312.88	K	Joback Method
tf	630.23	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.75	J/mol×K	1060.09	Joback Method
cpg	1431.94	J/mol×K	1102.22	Joback Method
cpg	1448.23	J/mol×K	1144.35	Joback Method
cpg	1462.72	J/mol×K	1186.48	Joback Method
cpg	1475.51	J/mol×K	1228.62	Joback Method
cpg	1486.70	J/mol×K	1270.75	Joback Method
cpg	1496.39	J/mol×K	1312.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348398&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