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

Inchi: InChI=1S/C27H43F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-33-27(32)22(3)30-

InchiKey: ZMRFLEFXODCPEW-UHFFFAOYSA-N

Formula: C27H43F2NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 467.63

Physical Properties

Property code	Value	Unit	Source
gf	-405.53	kJ/mol	Joback Method
hf	-1099.90	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	100.27	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	7.416		Crippen Method
mcvol	390.060	ml/mol	McGowan Method
pc	823.84	kPa	Joback Method
rinpol	3301.00		NIST Webbook
tb	1037.21	K	Joback Method
tc	1279.32	K	Joback Method
tf	618.96	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.67	J/mol×K	1037.21	Joback Method
cpg	1368.35	J/mol×K	1077.56	Joback Method
cpg	1384.29	J/mol×K	1117.91	Joback Method
cpg	1398.57	J/mol×K	1158.26	Joback Method
cpg	1411.28	J/mol×K	1198.61	Joback Method
cpg	1422.49	J/mol×K	1238.97	Joback Method
cpg	1432.28	J/mol×K	1279.32	Joback Method

Sources

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=U348397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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