D-Alanine, N-(3,4-difluorobenzoyl)-, eicosyl ester

Inchi: InChI=1S/C30H49F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-36-30(
InchiKey: FORQBRQKFMWJJF-UHFFFAOYSA-N
Formula: C30H49F2NO3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 509.71

Physical Properties

Property code	Value	Unit	Source
gf	-370.64	kJ/mol	Joback Method
hf	-1150.35	kJ/mol	Joback Method
hfus	78.84	kJ/mol	Joback Method
hvap	106.29	kJ/mol	Joback Method
log10ws	-10.66		Crippen Method
logp	8.668		Crippen Method
mcvol	432.330	ml/mol	McGowan Method
pc	708.46	kPa	Joback Method
rinpol	3556.00		NIST Webbook
rinpol	3556.00		NIST Webbook
tb	1100.87	K	Joback Method
tc	1377.70	K	Joback Method
tf	640.25	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1541.79	J/mol×K	1100.87	Joback Method
cpg	1561.38	J/mol×K	1147.01	Joback Method
cpg	1578.80	J/mol×K	1193.15	Joback Method
cpg	1594.19	J/mol×K	1239.28	Joback Method
cpg	1607.71	J/mol×K	1285.42	Joback Method
cpg	1619.52	J/mol×K	1331.56	Joback Method
cpg	1629.79	J/mol×K	1377.70	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=U348373&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