D-Alanine, N-(2,4-difluorobenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C27H43F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-33-27(32)22(2)3

InchiKey: VEHKLWZQMQPNEC-UHFFFAOYSA-N

Formula: C27H43F2NO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 467.63

Physical Properties

Property code	Value	Unit	Source
gf	-395.90	kJ/mol	Joback Method
hf	-1088.43	kJ/mol	Joback Method
hfus	71.07	kJ/mol	Joback Method
hvap	99.61	kJ/mol	Joback Method
log10ws	-9.41		Crippen Method
logp	7.498		Crippen Method
mcvol	390.060	ml/mol	McGowan Method
pc	830.98	kPa	Joback Method
rinpol	3192.00		NIST Webbook
rinpol	3192.00		NIST Webbook
tb	1032.23	K	Joback Method
tc	1272.86	K	Joback Method
tf	606.44	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.41	J/mol×K	1032.23	Joback Method
cpg	1369.26	J/mol×K	1072.33	Joback Method
cpg	1385.41	J/mol×K	1112.44	Joback Method
cpg	1399.97	J/mol×K	1152.54	Joback Method
cpg	1413.02	J/mol×K	1192.65	Joback Method
cpg	1424.65	J/mol×K	1232.75	Joback Method
cpg	1434.95	J/mol×K	1272.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348462&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

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