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

Inchi: InChI=1S/C22H33F2NO3/c1-3-4-5-6-7-8-9-10-11-12-15-28-22(27)17(2)25-21(26)18-13-1

InchiKey: DAEROLPNHMIWIR-UHFFFAOYSA-N

Formula: C22H33F2NO3

SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 397.50

Physical Properties

Property code	Value	Unit	Source
gf	-438.00	kJ/mol	Joback Method
hf	-985.23	kJ/mol	Joback Method
hfus	58.12	kJ/mol	Joback Method
hvap	88.48	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.547		Crippen Method
mcvol	319.610	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	917.83	K	Joback Method
tc	1124.13	K	Joback Method
tf	550.09	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.13	J/mol×K	917.83	Joback Method
cpg	1057.90	J/mol×K	952.21	Joback Method
cpg	1072.47	J/mol×K	986.60	Joback Method
cpg	1085.88	J/mol×K	1020.98	Joback Method
cpg	1098.18	J/mol×K	1055.36	Joback Method
cpg	1109.40	J/mol×K	1089.74	Joback Method
cpg	1119.60	J/mol×K	1124.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348367&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