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

Inchi: InChI=1S/C21H31F2NO3/c1-3-4-5-6-7-8-9-10-11-14-27-21(26)16(2)24-20(25)17-12-13-1

InchiKey: UZTZNLURTSFPKB-UHFFFAOYSA-N

Formula: C21H31F2NO3

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

Mol. weight [g/mol]: 383.47

Physical Properties

Property code	Value	Unit	Source
gf	-446.42	kJ/mol	Joback Method
hf	-964.59	kJ/mol	Joback Method
hfus	55.53	kJ/mol	Joback Method
hvap	86.26	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.157		Crippen Method
mcvol	305.520	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	2631.00		NIST Webbook
rinpol	2631.00		NIST Webbook
tb	894.95	K	Joback Method
tc	1097.50	K	Joback Method
tf	538.82	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.88	J/mol×K	894.95	Joback Method
cpg	997.32	J/mol×K	928.71	Joback Method
cpg	1011.62	J/mol×K	962.47	Joback Method
cpg	1024.83	J/mol×K	996.22	Joback Method
cpg	1036.97	J/mol×K	1029.98	Joback Method
cpg	1048.09	J/mol×K	1063.74	Joback Method
cpg	1058.23	J/mol×K	1097.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348366&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