«beta»-Alanine, N-(2,6-difluorobenzoyl)-, dodecyl ester

Inchi: InChI=1S/C22H33F2NO3/c1-2-3-4-5-6-7-8-9-10-11-17-28-20(26)15-16-25-22(27)21-18(2

InchiKey: ZDTVAHZRYITSPL-UHFFFAOYSA-N

Formula: C22H33F2NO3

SMILES: CCCCCCCCCCCCOC(=O)CCNC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 397.50

Physical Properties

Property code	Value	Unit	Source
gf	-435.56	kJ/mol	Joback Method
hf	-979.95	kJ/mol	Joback Method
hfus	61.64	kJ/mol	Joback Method
hvap	88.87	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.549		Crippen Method
mcvol	319.610	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	918.27	K	Joback Method
tc	1124.38	K	Joback Method
tf	565.09	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.67	J/mol×K	918.27	Joback Method
cpg	1057.46	J/mol×K	952.62	Joback Method
cpg	1072.06	J/mol×K	986.97	Joback Method
cpg	1085.51	J/mol×K	1021.32	Joback Method
cpg	1097.87	J/mol×K	1055.68	Joback Method
cpg	1109.17	J/mol×K	1090.03	Joback Method
cpg	1119.45	J/mol×K	1124.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321850&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