D-Alanine, N-(2,6-difluoro-3-methylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C23H35F2NO3/c1-4-5-6-7-8-9-10-11-12-13-16-29-23(28)18(3)26-22(27)20-19(

InchiKey: GSGSNNOZHXXEDH-UHFFFAOYSA-N

Formula: C23H35F2NO3

SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 411.53

Physical Properties

Property code	Value	Unit	Source
gf	-439.21	kJ/mol	Joback Method
hf	-1017.34	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	5.856		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	945.69	K	Joback Method
tc	1157.80	K	Joback Method
tf	573.88	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.29	J/mol×K	945.69	Joback Method
cpg	1118.32	J/mol×K	981.04	Joback Method
cpg	1133.06	J/mol×K	1016.39	Joback Method
cpg	1146.54	J/mol×K	1051.74	Joback Method
cpg	1158.81	J/mol×K	1087.09	Joback Method
cpg	1169.92	J/mol×K	1122.45	Joback Method
cpg	1179.90	J/mol×K	1157.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348393&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