D-Alanine, N-(2,5-difluorobenzoyl)-, tridecyl ester

Inchi: InChI=1S/C23H35F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-29-23(28)18(2)26-22(27)20-1
InchiKey: HANUNBRHPPYHGS-UHFFFAOYSA-N
Formula: C23H35F2NO3
SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 411.53

Physical Properties

Property code	Value	Unit	Source
gf	-429.58	kJ/mol	Joback Method
hf	-1005.87	kJ/mol	Joback Method
hfus	60.71	kJ/mol	Joback Method
hvap	90.71	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.937		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	940.71	K	Joback Method
tc	1151.69	K	Joback Method
tf	561.36	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.98	J/mol×K	940.71	Joback Method
cpg	1119.10	J/mol×K	975.87	Joback Method
cpg	1133.95	J/mol×K	1011.04	Joback Method
cpg	1147.57	J/mol×K	1046.20	Joback Method
cpg	1160.02	J/mol×K	1081.37	Joback Method
cpg	1171.34	J/mol×K	1116.53	Joback Method
cpg	1181.58	J/mol×K	1151.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348470&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

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