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

Inchi: InChI=1S/C24H37F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-17-30-24(29)19(3)27-23(28)21-

InchiKey: VDJDYVZUNYWMEF-UHFFFAOYSA-N

Formula: C24H37F2NO3

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

Mol. weight [g/mol]: 425.55

Physical Properties

Property code	Value	Unit	Source
gf	-430.79	kJ/mol	Joback Method
hf	-1037.98	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.246		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	979.01	kPa	Joback Method
rinpol	2996.00		NIST Webbook
rinpol	2996.00		NIST Webbook
tb	968.57	K	Joback Method
tc	1186.45	K	Joback Method
tf	585.15	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.70	J/mol×K	968.57	Joback Method
cpg	1180.10	J/mol×K	1004.88	Joback Method
cpg	1195.11	J/mol×K	1041.20	Joback Method
cpg	1208.78	J/mol×K	1077.51	Joback Method
cpg	1221.17	J/mol×K	1113.82	Joback Method
cpg	1232.33	J/mol×K	1150.14	Joback Method
cpg	1242.30	J/mol×K	1186.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348394&Units=SI

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