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

Inchi: InChI=1S/C26H41F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-32-26(31)21(3)29-25(

InchiKey: FFVOYKANDKNBHJ-UHFFFAOYSA-N

Formula: C26H41F2NO3

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

Mol. weight [g/mol]: 453.61

Physical Properties

Property code	Value	Unit	Source
gf	-413.95	kJ/mol	Joback Method
hf	-1079.26	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	98.05	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	7.026		Crippen Method
mcvol	375.970	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinpol	3202.00		NIST Webbook
rinpol	3202.00		NIST Webbook
tb	1014.33	K	Joback Method
tc	1247.12	K	Joback Method
tf	607.69	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.93	J/mol×K	1014.33	Joback Method
cpg	1305.15	J/mol×K	1053.13	Joback Method
cpg	1320.77	J/mol×K	1091.93	Joback Method
cpg	1334.84	J/mol×K	1130.73	Joback Method
cpg	1347.45	J/mol×K	1169.52	Joback Method
cpg	1358.66	J/mol×K	1208.32	Joback Method
cpg	1368.54	J/mol×K	1247.12	Joback Method

Sources

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=U348396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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