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

Inchi: InChI=1S/C24H37F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-30-24(29)19(2)27-23(28)2

InchiKey: AXULAGMQFMUWGZ-UHFFFAOYSA-N

Formula: C24H37F2NO3

SMILES: CCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 425.55

Physical Properties

Property code	Value	Unit	Source
gf	-421.16	kJ/mol	Joback Method
hf	-1026.51	kJ/mol	Joback Method
hfus	63.30	kJ/mol	Joback Method
hvap	92.93	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	6.327		Crippen Method
mcvol	347.790	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	963.59	K	Joback Method
tc	1180.27	K	Joback Method
tf	572.63	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1164.39	J/mol×K	963.59	Joback Method
cpg	1180.88	J/mol×K	999.70	Joback Method
cpg	1196.02	J/mol×K	1035.82	Joback Method
cpg	1209.86	J/mol×K	1071.93	Joback Method
cpg	1222.46	J/mol×K	1108.04	Joback Method
cpg	1233.87	J/mol×K	1144.16	Joback Method
cpg	1244.14	J/mol×K	1180.27	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=U348471&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