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

Inchi: InChI=1S/C25H39F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-31-25(30)20(2)28-24(2

InchiKey: NXCBUWSKEOEYCR-UHFFFAOYSA-N

Formula: C25H39F2NO3

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

Mol. weight [g/mol]: 439.58

Physical Properties

Property code	Value	Unit	Source
gf	-412.74	kJ/mol	Joback Method
hf	-1047.15	kJ/mol	Joback Method
hfus	65.89	kJ/mol	Joback Method
hvap	95.16	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	6.718		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	931.21	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	986.47	K	Joback Method
tc	1209.93	K	Joback Method
tf	583.90	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.29	J/mol×K	986.47	Joback Method
cpg	1243.20	J/mol×K	1023.71	Joback Method
cpg	1258.65	J/mol×K	1060.96	Joback Method
cpg	1272.72	J/mol×K	1098.20	Joback Method
cpg	1285.46	J/mol×K	1135.45	Joback Method
cpg	1296.95	J/mol×K	1172.69	Joback Method
cpg	1307.25	J/mol×K	1209.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348472&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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