«beta»-Alanine, N-(2,6-difluorobenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C25H39F2NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-31-23(29)18-19-28-25(3

InchiKey: LURMHQOIYFPPNG-UHFFFAOYSA-N

Formula: C25H39F2NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CCNC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 439.58

Physical Properties

Property code	Value	Unit	Source
gf	-410.30	kJ/mol	Joback Method
hf	-1041.87	kJ/mol	Joback Method
hfus	69.41	kJ/mol	Joback Method
hvap	95.55	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	6.719		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
tb	986.91	K	Joback Method
tc	1211.39	K	Joback Method
tf	598.90	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.94	J/mol×K	986.91	Joback Method
cpg	1242.97	J/mol×K	1024.32	Joback Method
cpg	1258.56	J/mol×K	1061.74	Joback Method
cpg	1272.77	J/mol×K	1099.15	Joback Method
cpg	1285.65	J/mol×K	1136.57	Joback Method
cpg	1297.28	J/mol×K	1173.98	Joback Method
cpg	1307.72	J/mol×K	1211.39	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=U321852&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume