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

Inchi: InChI=1S/C20H29F2NO3/c1-2-3-4-5-6-7-8-9-15-26-18(24)13-14-23-20(25)19-16(21)11-1

InchiKey: AOJOMIAVCWRIEW-UHFFFAOYSA-N

Formula: C20H29F2NO3

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

Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
gf	-452.40	kJ/mol	Joback Method
hf	-938.67	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	4.769		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	872.51	K	Joback Method
tc	1071.28	K	Joback Method
tf	542.55	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.78	J/mol×K	872.51	Joback Method
cpg	936.86	J/mol×K	905.64	Joback Method
cpg	950.88	J/mol×K	938.77	Joback Method
cpg	963.87	J/mol×K	971.90	Joback Method
cpg	975.87	J/mol×K	1005.02	Joback Method
cpg	986.90	J/mol×K	1038.15	Joback Method
cpg	997.01	J/mol×K	1071.28	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=U321848&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