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

Inchi: InChI=1S/C16H21F2NO3/c1-2-3-4-5-11-22-14(20)9-10-19-16(21)15-12(17)7-6-8-13(15)1

InchiKey: PCVORLYYYGRNKI-UHFFFAOYSA-N

Formula: C16H21F2NO3

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

Mol. weight [g/mol]: 313.34

Physical Properties

Property code	Value	Unit	Source
gf	-486.08	kJ/mol	Joback Method
hf	-856.11	kJ/mol	Joback Method
hfus	46.10	kJ/mol	Joback Method
hvap	75.51	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.208		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
rinpol	2270.00		NIST Webbook
tb	780.99	K	Joback Method
tc	974.53	K	Joback Method
tf	497.47	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.25	J/mol×K	780.99	Joback Method
cpg	704.97	J/mol×K	813.25	Joback Method
cpg	717.81	J/mol×K	845.50	Joback Method
cpg	729.79	J/mol×K	877.76	Joback Method
cpg	740.93	J/mol×K	910.01	Joback Method
cpg	751.25	J/mol×K	942.27	Joback Method
cpg	760.78	J/mol×K	974.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321844&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