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

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

InchiKey: RQCUCCOQPPFQNQ-UHFFFAOYSA-N

Formula: C16H21F2NO3

SMILES: CC(C)CCCOC(=O)CCNC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 313.34

Physical Properties

Property code	Value	Unit	Source
gf	-488.52	kJ/mol	Joback Method
hf	-861.39	kJ/mol	Joback Method
hfus	42.58	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.064		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	780.55	K	Joback Method
tc	976.25	K	Joback Method
tf	482.47	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.81	J/mol×K	780.55	Joback Method
cpg	705.69	J/mol×K	813.17	Joback Method
cpg	718.66	J/mol×K	845.78	Joback Method
cpg	730.73	J/mol×K	878.40	Joback Method
cpg	741.94	J/mol×K	911.02	Joback Method
cpg	752.31	J/mol×K	943.63	Joback Method
cpg	761.85	J/mol×K	976.25	Joback Method

Sources

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=U321843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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