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

Inchi: InChI=1S/C17H23F2NO3/c1-2-3-4-5-6-12-23-15(21)10-11-20-17(22)16-13(18)8-7-9-14(1

InchiKey: IUFCJLORSONGBC-UHFFFAOYSA-N

Formula: C17H23F2NO3

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

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-477.66	kJ/mol	Joback Method
hf	-876.75	kJ/mol	Joback Method
hfus	48.69	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.598		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	803.87	K	Joback Method
tc	997.68	K	Joback Method
tf	508.74	K	Joback Method
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.56	J/mol×K	803.87	Joback Method
cpg	761.64	J/mol×K	836.17	Joback Method
cpg	774.79	J/mol×K	868.47	Joback Method
cpg	787.05	J/mol×K	900.78	Joback Method
cpg	798.43	J/mol×K	933.08	Joback Method
cpg	808.97	J/mol×K	965.38	Joback Method
cpg	818.67	J/mol×K	997.68	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=U321845&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