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

Inchi: InChI=1S/C12H13F2NO3/c1-2-18-10(16)6-7-15-12(17)11-8(13)4-3-5-9(11)14/h3-5H,2,6-

InchiKey: DCPLMPSRUHFYLF-UHFFFAOYSA-N

Formula: C12H13F2NO3

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

Mol. weight [g/mol]: 257.23

Physical Properties

Property code	Value	Unit	Source
gf	-519.76	kJ/mol	Joback Method
hf	-773.55	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.648		Crippen Method
mcvol	178.710	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1866.00		NIST Webbook
tb	689.47	K	Joback Method
tc	887.43	K	Joback Method
tf	452.39	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.81	J/mol×K	689.47	Joback Method
cpg	488.76	J/mol×K	722.46	Joback Method
cpg	499.98	J/mol×K	755.46	Joback Method
cpg	510.47	J/mol×K	788.45	Joback Method
cpg	520.25	J/mol×K	821.45	Joback Method
cpg	529.34	J/mol×K	854.44	Joback Method
cpg	537.73	J/mol×K	887.43	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=U321839&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