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

Inchi: InChI=1S/C14H17F2NO3/c1-2-3-9-20-12(18)7-8-17-14(19)13-10(15)5-4-6-11(13)16/h4-6

InchiKey: UDUQRHSRDFZCMF-UHFFFAOYSA-N

Formula: C14H17F2NO3

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

Mol. weight [g/mol]: 285.29

Physical Properties

Property code	Value	Unit	Source
gf	-502.92	kJ/mol	Joback Method
hf	-814.83	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	71.06	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.428		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	735.23	K	Joback Method
tc	929.97	K	Joback Method
tf	474.93	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.71	J/mol×K	735.23	Joback Method
cpg	594.64	J/mol×K	767.69	Joback Method
cpg	606.76	J/mol×K	800.14	Joback Method
cpg	618.09	J/mol×K	832.60	Joback Method
cpg	628.65	J/mol×K	865.06	Joback Method
cpg	638.44	J/mol×K	897.51	Joback Method
cpg	647.49	J/mol×K	929.97	Joback Method

Sources

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=U321841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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