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

Inchi: InChI=1S/C15H19F2NO3/c1-2-3-4-10-21-13(19)8-9-18-15(20)14-11(16)6-5-7-12(14)17/h

InchiKey: IEBGJBALOIZJOI-UHFFFAOYSA-N

Formula: C15H19F2NO3

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

Mol. weight [g/mol]: 299.31

Physical Properties

Property code	Value	Unit	Source
gf	-494.50	kJ/mol	Joback Method
hf	-835.47	kJ/mol	Joback Method
hfus	43.51	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	2.818		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	2166.00		NIST Webbook
tb	758.11	K	Joback Method
tc	951.97	K	Joback Method
tf	486.20	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.94	J/mol×K	758.11	Joback Method
cpg	649.29	J/mol×K	790.42	Joback Method
cpg	661.79	J/mol×K	822.73	Joback Method
cpg	673.46	J/mol×K	855.04	Joback Method
cpg	684.32	J/mol×K	887.35	Joback Method
cpg	694.40	J/mol×K	919.66	Joback Method
cpg	703.71	J/mol×K	951.97	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=U321842&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

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