D-Alanine, N-(3,4-difluorobenzoyl)-, pentyl ester

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

InchiKey: JMKRYJDFZZUCCH-UHFFFAOYSA-N

Formula: C15H19F2NO3

SMILES: CCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 299.31

Physical Properties

Property code	Value	Unit	Source
gf	-496.94	kJ/mol	Joback Method
hf	-840.75	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	2.817		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	757.67	K	Joback Method
tc	953.98	K	Joback Method
tf	471.20	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.50	J/mol×K	757.67	Joback Method
cpg	650.02	J/mol×K	790.39	Joback Method
cpg	662.67	J/mol×K	823.11	Joback Method
cpg	674.46	J/mol×K	855.83	Joback Method
cpg	685.41	J/mol×K	888.55	Joback Method
cpg	695.55	J/mol×K	921.27	Joback Method
cpg	704.88	J/mol×K	953.98	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=U348361&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