D-alanine, n-(2,4-difluorobenzoyl)-, pentyl ester

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

InchiKey: FDJBPNBSHSGEGU-UHFFFAOYSA-N

Formula: C15H19F2NO3

SMILES: CCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
hfus	39.99	kJ/mol	Joback Method
logp	2.817		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	585.33	K	Cheméo Relay (1.0)
tf	344.66	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348459&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point