D-Alanine, N-(2,4-difluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C13H15F2NO3/c1-3-6-19-13(18)8(2)16-12(17)10-5-4-9(14)7-11(10)15/h4-5,7-8

InchiKey: YVVCZVOJBDCPAI-UHFFFAOYSA-N

Formula: C13H15F2NO3

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

Mol. weight [g/mol]: 271.26

Physical Properties

Property code	Value	Unit	Source
gf	-513.78	kJ/mol	Joback Method
hf	-799.47	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.036		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1787.00		NIST Webbook
tb	711.91	K	Joback Method
tc	911.04	K	Joback Method
tf	448.66	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.20	J/mol×K	711.91	Joback Method
cpg	541.88	J/mol×K	745.10	Joback Method
cpg	553.75	J/mol×K	778.29	Joback Method
cpg	564.84	J/mol×K	811.48	Joback Method
cpg	575.15	J/mol×K	844.66	Joback Method
cpg	584.69	J/mol×K	877.85	Joback Method
cpg	593.49	J/mol×K	911.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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