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

Inchi: InChI=1S/C14H17F2NO3/c1-3-4-7-20-14(19)9(2)17-13(18)11-6-5-10(15)8-12(11)16/h5-6
InchiKey: BWRIFFQTVGJBJD-UHFFFAOYSA-N
Formula: C14H17F2NO3
SMILES: CCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 285.29

Physical Properties

Property code	Value	Unit	Source
gf	-505.36	kJ/mol	Joback Method
hf	-820.11	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	70.67	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.426		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	734.79	K	Joback Method
tc	932.26	K	Joback Method
tf	459.93	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.27	J/mol×K	734.79	Joback Method
cpg	595.40	J/mol×K	767.70	Joback Method
cpg	607.68	J/mol×K	800.61	Joback Method
cpg	619.14	J/mol×K	833.53	Joback Method
cpg	629.80	J/mol×K	866.44	Joback Method
cpg	639.66	J/mol×K	899.35	Joback Method
cpg	648.75	J/mol×K	932.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348458&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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