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

Inchi: InChI=1S/C16H21F2NO3/c1-10(2)5-4-8-22-16(21)11(3)19-15(20)13-7-6-12(17)9-14(13)1

InchiKey: ZTBBDPZZNOWUJD-UHFFFAOYSA-N

Formula: C16H21F2NO3

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

Mol. weight [g/mol]: 313.34

Physical Properties

Property code	Value	Unit	Source
gf	-490.96	kJ/mol	Joback Method
hf	-866.67	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.062		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	780.11	K	Joback Method
tc	978.11	K	Joback Method
tf	467.47	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.37	J/mol×K	780.11	Joback Method
cpg	706.41	J/mol×K	813.11	Joback Method
cpg	719.51	J/mol×K	846.11	Joback Method
cpg	731.70	J/mol×K	879.11	Joback Method
cpg	742.98	J/mol×K	912.11	Joback Method
cpg	753.39	J/mol×K	945.11	Joback Method
cpg	762.94	J/mol×K	978.11	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=U348460&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