D-Alanine, N-(2,6-difluoro-3-methylbenzoyl)-, isohexyl ester

Inchi: InChI=1S/C17H23F2NO3/c1-10(2)6-5-9-23-17(22)12(4)20-16(21)14-13(18)8-7-11(3)15(1

InchiKey: MZMXUHSJHZMWKP-UHFFFAOYSA-N

Formula: C17H23F2NO3

SMILES: Cc1ccc(F)c(C(=O)NC(C)C(=O)OCCCC(C)C)c1F

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-492.17	kJ/mol	Joback Method
hf	-898.78	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	77.63	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	3.371		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	807.97	K	Joback Method
tc	1006.49	K	Joback Method
tf	491.26	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.77	J/mol×K	807.97	Joback Method
cpg	762.04	J/mol×K	841.06	Joback Method
cpg	775.33	J/mol×K	874.14	Joback Method
cpg	787.68	J/mol×K	907.23	Joback Method
cpg	799.09	J/mol×K	940.31	Joback Method
cpg	809.58	J/mol×K	973.40	Joback Method
cpg	819.19	J/mol×K	1006.49	Joback Method

Sources

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=U348388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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