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

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

InchiKey: PYJOGUVBBFDTNK-UHFFFAOYSA-N

Formula: C17H23F2NO3

SMILES: CCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-489.73	kJ/mol	Joback Method
hf	-893.50	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	3.515		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
pc	1569.72	kPa	Joback Method
rinpol	2283.00		NIST Webbook
tb	808.41	K	Joback Method
tc	1004.93	K	Joback Method
tf	506.26	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.22	J/mol×K	808.41	Joback Method
cpg	761.35	J/mol×K	841.16	Joback Method
cpg	774.53	J/mol×K	873.92	Joback Method
cpg	786.80	J/mol×K	906.67	Joback Method
cpg	798.15	J/mol×K	939.43	Joback Method
cpg	808.62	J/mol×K	972.18	Joback Method
cpg	818.23	J/mol×K	1004.93	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=U348389&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