D-Alanine, N-(3,4-difluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H27F2NO3/c1-3-4-5-6-7-8-9-12-25-19(24)14(2)22-18(23)15-10-11-16(20)1

InchiKey: IQKLOSKFRZEFTM-UHFFFAOYSA-N

Formula: C19H27F2NO3

SMILES: CCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1

Mol. weight [g/mol]: 355.42

Physical Properties

Property code	Value	Unit	Source
gf	-463.26	kJ/mol	Joback Method
hf	-923.31	kJ/mol	Joback Method
hfus	50.35	kJ/mol	Joback Method
hvap	81.80	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.377		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	849.19	K	Joback Method
tc	1046.80	K	Joback Method
tf	516.28	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.42	J/mol×K	849.19	Joback Method
cpg	878.25	J/mol×K	882.12	Joback Method
cpg	892.04	J/mol×K	915.06	Joback Method
cpg	904.83	J/mol×K	947.99	Joback Method
cpg	916.65	J/mol×K	980.93	Joback Method
cpg	927.52	J/mol×K	1013.86	Joback Method
cpg	937.49	J/mol×K	1046.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348364&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