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

Inchi: InChI=1S/C20H29F2NO3/c1-4-5-6-7-8-9-10-13-26-20(25)15(3)23-19(24)17-16(21)12-11-

InchiKey: ZPJQCSAAXAPUEP-UHFFFAOYSA-N

Formula: C20H29F2NO3

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

Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
gf	-464.47	kJ/mol	Joback Method
hf	-955.42	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	4.685		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	877.05	K	Joback Method
tc	1077.67	K	Joback Method
tf	540.07	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.53	J/mol×K	877.05	Joback Method
cpg	936.58	J/mol×K	910.49	Joback Method
cpg	950.55	J/mol×K	943.92	Joback Method
cpg	963.46	J/mol×K	977.36	Joback Method
cpg	975.33	J/mol×K	1010.80	Joback Method
cpg	986.21	J/mol×K	1044.24	Joback Method
cpg	996.10	J/mol×K	1077.67	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=U348390&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