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

Inchi: InChI=1S/C29H47F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-35-29(34)
InchiKey: MUXWYTXZJGZPOK-UHFFFAOYSA-N
Formula: C29H47F2NO3
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 495.69

Physical Properties

Property code	Value	Unit	Source
gf	-379.06	kJ/mol	Joback Method
hf	-1129.71	kJ/mol	Joback Method
hfus	76.25	kJ/mol	Joback Method
hvap	104.06	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	8.278		Crippen Method
mcvol	418.240	ml/mol	McGowan Method
pc	746.11	kPa	Joback Method
rinpol	3397.00		NIST Webbook
rinpol	3397.00		NIST Webbook
tb	1077.99	K	Joback Method
tc	1341.21	K	Joback Method
tf	628.98	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1478.02	J/mol×K	1077.99	Joback Method
cpg	1496.98	J/mol×K	1121.86	Joback Method
cpg	1513.94	J/mol×K	1165.73	Joback Method
cpg	1529.04	J/mol×K	1209.60	Joback Method
cpg	1542.40	J/mol×K	1253.47	Joback Method
cpg	1554.15	J/mol×K	1297.34	Joback Method
cpg	1564.43	J/mol×K	1341.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348464&Units=SI

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