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

Inchi: InChI=1S/C26H41F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-32-26(31)21(2)29-2

InchiKey: HAZVJBJPASAMTQ-UHFFFAOYSA-N

Formula: C26H41F2NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F

Mol. weight [g/mol]: 453.61

Physical Properties

Property code	Value	Unit	Source
gf	-404.32	kJ/mol	Joback Method
hf	-1067.79	kJ/mol	Joback Method
hfus	68.48	kJ/mol	Joback Method
hvap	97.39	kJ/mol	Joback Method
log10ws	-8.99		Crippen Method
logp	7.108		Crippen Method
mcvol	375.970	ml/mol	McGowan Method
pc	878.96	kPa	Joback Method
rinpol	3089.00		NIST Webbook
tb	1009.35	K	Joback Method
tc	1240.77	K	Joback Method
tf	595.17	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1288.65	J/mol×K	1009.35	Joback Method
cpg	1306.00	J/mol×K	1047.92	Joback Method
cpg	1321.79	J/mol×K	1086.49	Joback Method
cpg	1336.10	J/mol×K	1125.06	Joback Method
cpg	1349.00	J/mol×K	1163.63	Joback Method
cpg	1360.56	J/mol×K	1202.20	Joback Method
cpg	1370.86	J/mol×K	1240.77	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=U348461&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