D-Alanine, N-(2,5-difluorobenzoyl)-, octadecyl ester

Inchi: InChI=1S/C28H45F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-34-28(33)23(
InchiKey: LQTQLOJTHFRGRZ-UHFFFAOYSA-N
Formula: C28H45F2NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 481.66

Physical Properties

Property code	Value	Unit	Source
gf	-387.48	kJ/mol	Joback Method
hf	-1109.07	kJ/mol	Joback Method
hfus	73.66	kJ/mol	Joback Method
hvap	101.84	kJ/mol	Joback Method
log10ws	-9.83		Crippen Method
logp	7.888		Crippen Method
mcvol	404.150	ml/mol	McGowan Method
pc	786.83	kPa	Joback Method
rinpol	3321.00		NIST Webbook
rinpol	3321.00		NIST Webbook
tb	1055.11	K	Joback Method
tc	1306.31	K	Joback Method
tf	617.71	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1414.55	J/mol×K	1055.11	Joback Method
cpg	1432.93	J/mol×K	1096.98	Joback Method
cpg	1449.47	J/mol×K	1138.84	Joback Method
cpg	1464.29	J/mol×K	1180.71	Joback Method
cpg	1477.50	J/mol×K	1222.57	Joback Method
cpg	1489.19	J/mol×K	1264.44	Joback Method
cpg	1499.48	J/mol×K	1306.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348475&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