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

Inchi: InChI=1S/C25H39F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-31-25(30)20(3)28-24(29)
InchiKey: DVUCLMCSYZFBOY-UHFFFAOYSA-N
Formula: C25H39F2NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 439.58

Physical Properties

Property code	Value	Unit	Source
gf	-422.37	kJ/mol	Joback Method
hf	-1058.62	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	6.636		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	922.74	kPa	Joback Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
tb	991.45	K	Joback Method
tc	1216.20	K	Joback Method
tf	596.42	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.60	J/mol×K	991.45	Joback Method
cpg	1242.39	J/mol×K	1028.91	Joback Method
cpg	1257.69	J/mol×K	1066.37	Joback Method
cpg	1271.56	J/mol×K	1103.82	Joback Method
cpg	1284.07	J/mol×K	1141.28	Joback Method
cpg	1295.26	J/mol×K	1178.74	Joback Method
cpg	1305.20	J/mol×K	1216.20	Joback Method

Sources

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=U348395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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