D-Alanine, N-(3-anisoyl)-, undecyl ester

Inchi: InChI=1S/C22H35NO4/c1-4-5-6-7-8-9-10-11-12-16-27-22(25)18(2)23-21(24)19-14-13-15
InchiKey: BTFFXSUQXKHSAQ-UHFFFAOYSA-N
Formula: C22H35NO4
SMILES: CCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
gf	-143.75	kJ/mol	Joback Method
hf	-713.76	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	4.888		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2939.00		NIST Webbook
rinpol	2939.00		NIST Webbook
tb	936.73	K	Joback Method
tc	1148.47	K	Joback Method
tf	558.62	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.99	J/mol×K	936.73	Joback Method
cpg	1073.72	J/mol×K	972.02	Joback Method
cpg	1088.10	J/mol×K	1007.31	Joback Method
cpg	1101.18	J/mol×K	1042.60	Joback Method
cpg	1112.98	J/mol×K	1077.89	Joback Method
cpg	1123.54	J/mol×K	1113.18	Joback Method
cpg	1132.89	J/mol×K	1148.47	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=U354049&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