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

Inchi: InChI=1S/C27H45NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-32-27(30)23(2)28-26
InchiKey: LATZXZKSLZIHBK-UHFFFAOYSA-N
Formula: C27H45NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
gf	-101.65	kJ/mol	Joback Method
hf	-816.96	kJ/mol	Joback Method
hfus	66.49	kJ/mol	Joback Method
hvap	102.99	kJ/mol	Joback Method
log10ws	-8.45		Crippen Method
logp	6.838		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
pc	874.80	kPa	Joback Method
rinpol	3455.00		NIST Webbook
tb	1051.13	K	Joback Method
tc	1292.61	K	Joback Method
tf	614.97	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1367.46	J/mol×K	1051.13	Joback Method
cpg	1384.38	J/mol×K	1091.38	Joback Method
cpg	1399.46	J/mol×K	1131.62	Joback Method
cpg	1412.76	J/mol×K	1171.87	Joback Method
cpg	1424.37	J/mol×K	1212.12	Joback Method
cpg	1434.36	J/mol×K	1252.37	Joback Method
cpg	1442.81	J/mol×K	1292.61	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=U354054&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