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

Inchi: InChI=1S/C23H37NO4/c1-4-5-6-7-8-9-10-11-12-13-17-28-23(26)19(2)24-22(25)20-15-14
InchiKey: PDVBOGKZQQAVJF-UHFFFAOYSA-N
Formula: C23H37NO4
SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 391.54

Physical Properties

Property code	Value	Unit	Source
gf	-135.33	kJ/mol	Joback Method
hf	-734.40	kJ/mol	Joback Method
hfus	56.13	kJ/mol	Joback Method
hvap	94.09	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.278		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		NIST Webbook
tb	959.61	K	Joback Method
tc	1175.17	K	Joback Method
tf	569.89	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.01	J/mol×K	959.61	Joback Method
cpg	1134.94	J/mol×K	995.54	Joback Method
cpg	1149.45	J/mol×K	1031.46	Joback Method
cpg	1162.58	J/mol×K	1067.39	Joback Method
cpg	1174.37	J/mol×K	1103.32	Joback Method
cpg	1184.87	J/mol×K	1139.25	Joback Method
cpg	1194.11	J/mol×K	1175.17	Joback Method

Sources

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=U354050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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