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

Inchi: InChI=1S/C24H39NO4/c1-4-5-6-7-8-9-10-11-12-13-14-18-29-24(27)20(2)25-23(26)21-16
InchiKey: CBVAMWGYCPCKPD-UHFFFAOYSA-N
Formula: C24H39NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 405.57

Physical Properties

Property code	Value	Unit	Source
gf	-126.91	kJ/mol	Joback Method
hf	-755.04	kJ/mol	Joback Method
hfus	58.72	kJ/mol	Joback Method
hvap	96.32	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	5.668		Crippen Method
mcvol	350.120	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	3143.00		NIST Webbook
tb	982.49	K	Joback Method
tc	1202.86	K	Joback Method
tf	581.16	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.53	J/mol×K	982.49	Joback Method
cpg	1196.67	J/mol×K	1019.22	Joback Method
cpg	1211.31	J/mol×K	1055.95	Joback Method
cpg	1224.49	J/mol×K	1092.68	Joback Method
cpg	1236.26	J/mol×K	1129.40	Joback Method
cpg	1246.67	J/mol×K	1166.13	Joback Method
cpg	1255.76	J/mol×K	1202.86	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=U354051&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

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