D-Alanine, N-(4-anisoyl)-, decyl ester

Inchi: InChI=1S/C21H33NO4/c1-4-5-6-7-8-9-10-11-16-26-21(24)17(2)22-20(23)18-12-14-19(25
InchiKey: LGTSRMGLHRQYAQ-UHFFFAOYSA-N
Formula: C21H33NO4
SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
gf	-152.17	kJ/mol	Joback Method
hf	-693.12	kJ/mol	Joback Method
hfus	50.95	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.497		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2849.00		NIST Webbook
tb	913.85	K	Joback Method
tc	1122.70	K	Joback Method
tf	547.35	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.49	J/mol×K	913.85	Joback Method
cpg	1013.04	J/mol×K	948.66	Joback Method
cpg	1027.30	J/mol×K	983.47	Joback Method
cpg	1040.32	J/mol×K	1018.27	Joback Method
cpg	1052.11	J/mol×K	1053.08	Joback Method
cpg	1062.71	J/mol×K	1087.89	Joback Method
cpg	1072.16	J/mol×K	1122.70	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=U348494&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