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

Inchi: InChI=1S/C13H17NO4/c1-4-18-13(16)9(2)14-12(15)10-5-7-11(17-3)8-6-10/h5-9H,4H2,1-
InchiKey: NXDSRAXOGAUMGJ-UHFFFAOYSA-N
Formula: C13H17NO4
SMILES: CCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	-219.53	kJ/mol	Joback Method
hf	-528.00	kJ/mol	Joback Method
hfus	30.23	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	1.377		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	730.81	K	Joback Method
tc	942.95	K	Joback Method
tf	457.19	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.55	J/mol×K	730.81	Joback Method
cpg	554.20	J/mol×K	766.17	Joback Method
cpg	566.90	J/mol×K	801.52	Joback Method
cpg	578.66	J/mol×K	836.88	Joback Method
cpg	589.48	J/mol×K	872.24	Joback Method
cpg	599.37	J/mol×K	907.59	Joback Method
cpg	608.35	J/mol×K	942.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348485&Units=SI
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

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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