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

Inchi: InChI=1S/C14H19NO4/c1-4-9-19-14(17)10(2)15-13(16)11-5-7-12(18-3)8-6-11/h5-8,10H,
InchiKey: DQERPFAVOPCNLV-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-211.11	kJ/mol	Joback Method
hf	-548.64	kJ/mol	Joback Method
hfus	32.82	kJ/mol	Joback Method
hvap	74.06	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	1.767		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	2105.00		NIST Webbook
tb	753.69	K	Joback Method
tc	963.31	K	Joback Method
tf	468.46	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.38	J/mol×K	753.69	Joback Method
cpg	608.39	J/mol×K	788.63	Joback Method
cpg	621.42	J/mol×K	823.56	Joback Method
cpg	633.47	J/mol×K	858.50	Joback Method
cpg	644.55	J/mol×K	893.44	Joback Method
cpg	654.68	J/mol×K	928.37	Joback Method
cpg	663.87	J/mol×K	963.31	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=U348486&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