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

Inchi: InChI=1S/C16H23NO4/c1-4-5-6-10-21-16(19)12(2)17-15(18)13-8-7-9-14(11-13)20-3/h7-9
InchiKey: BBRWJFVTPPAVAU-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-194.27	kJ/mol	Joback Method
hf	-589.92	kJ/mol	Joback Method
hfus	38.00	kJ/mol	Joback Method
hvap	78.51	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.547		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	799.45	K	Joback Method
tc	1005.61	K	Joback Method
tf	491.00	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.23	J/mol×K	799.45	Joback Method
cpg	719.81	J/mol×K	833.81	Joback Method
cpg	733.34	J/mol×K	868.17	Joback Method
cpg	745.82	J/mol×K	902.53	Joback Method
cpg	757.27	J/mol×K	936.89	Joback Method
cpg	767.71	J/mol×K	971.25	Joback Method
cpg	777.16	J/mol×K	1005.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354044&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