«beta»-Alanine, N-(4-methoxybenzoyl)-, undecyl ester

Inchi: InChI=1S/C22H35NO4/c1-3-4-5-6-7-8-9-10-11-18-27-21(24)16-17-23-22(25)19-12-14-20

InchiKey: GCXOEGHATBAOSC-UHFFFAOYSA-N

Formula: C22H35NO4

SMILES: CCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(OC)cc1

Mol. weight [g/mol]: 377.52

Physical Properties

Property code	Value	Unit	Source
gf	-141.31	kJ/mol	Joback Method
hf	-708.48	kJ/mol	Joback Method
hfus	57.06	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.889		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
tb	937.17	K	Joback Method
tc	1148.38	K	Joback Method
tf	573.62	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.55	J/mol×K	937.17	Joback Method
cpg	1073.28	J/mol×K	972.37	Joback Method
cpg	1087.68	J/mol×K	1007.57	Joback Method
cpg	1100.79	J/mol×K	1042.78	Joback Method
cpg	1112.65	J/mol×K	1077.98	Joback Method
cpg	1123.28	J/mol×K	1113.18	Joback Method
cpg	1132.73	J/mol×K	1148.38	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=U321827&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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