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

Inchi: InChI=1S/C16H23NO4/c1-3-4-5-12-21-15(18)10-11-17-16(19)13-6-8-14(20-2)9-7-13/h6-9

InchiKey: DPJNZOLTRIRMCN-UHFFFAOYSA-N

Formula: C16H23NO4

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

Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-191.83	kJ/mol	Joback Method
hf	-584.64	kJ/mol	Joback Method
hfus	41.52	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.548		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	799.89	K	Joback Method
tc	1003.51	K	Joback Method
tf	506.00	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.68	J/mol×K	799.89	Joback Method
cpg	719.08	J/mol×K	833.83	Joback Method
cpg	732.46	J/mol×K	867.76	Joback Method
cpg	744.84	J/mol×K	901.70	Joback Method
cpg	756.23	J/mol×K	935.64	Joback Method
cpg	766.63	J/mol×K	969.57	Joback Method
cpg	776.08	J/mol×K	1003.51	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=U321823&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