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

Inchi: InChI=1S/C13H17NO4/c1-3-18-12(15)8-9-14-13(16)10-4-6-11(17-2)7-5-10/h4-7H,3,8-9H

InchiKey: RDVGDIITDFDTLE-UHFFFAOYSA-N

Formula: C13H17NO4

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

Mol. weight [g/mol]: 251.28

Physical Properties

Property code	Value	Unit	Source
gf	-217.09	kJ/mol	Joback Method
hf	-522.72	kJ/mol	Joback Method
hfus	33.75	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.378		Crippen Method
mcvol	195.130	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook
tb	731.25	K	Joback Method
tc	939.96	K	Joback Method
tf	472.19	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.99	J/mol×K	731.25	Joback Method
cpg	553.40	J/mol×K	766.04	Joback Method
cpg	565.91	J/mol×K	800.82	Joback Method
cpg	577.51	J/mol×K	835.61	Joback Method
cpg	588.22	J/mol×K	870.39	Joback Method
cpg	598.04	J/mol×K	905.18	Joback Method
cpg	606.99	J/mol×K	939.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321820&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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