«beta»-Alanine, N-(3-methoxybenzoyl)-, propyl ester

Inchi: InChI=1S/C14H19NO4/c1-3-9-19-13(16)7-8-15-14(17)11-5-4-6-12(10-11)18-2/h4-6,10H,
InchiKey: NLCCEAVLQQGPIS-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-208.67	kJ/mol	Joback Method
hf	-543.36	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	1.768		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	754.13	K	Joback Method
tc	960.61	K	Joback Method
tf	483.46	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.81	J/mol×K	754.13	Joback Method
cpg	607.61	J/mol×K	788.54	Joback Method
cpg	620.46	J/mol×K	822.96	Joback Method
cpg	632.37	J/mol×K	857.37	Joback Method
cpg	643.35	J/mol×K	891.79	Joback Method
cpg	653.42	J/mol×K	926.20	Joback Method
cpg	662.58	J/mol×K	960.61	Joback Method

Sources

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=U321704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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