

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

Inchi:	InChI=1S/C14H19NO4/c1-3-10-19-13(16)8-9-15-14(17)11-4-6-12(18-2)7-5-11/h4-7H,3,8
InchiKey:	QKUFGIYKIOUVNE-UHFFFAOYSA-N
Formula:	C14H19NO4
SMILES:	CCCOC(=O)CCNC(=O)c1ccc(OC)cc1
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	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	754.13	K	Joback Method
tc	960.61	K	Joback Method
tf	483.46	K	Joback Method
vc	0.794	m ³ /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=U321821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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