

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

Inchi:	InChI=1S/C15H21NO4/c1-3-4-10-20-14(17)8-9-16-15(18)12-6-5-7-13(11-12)19-2/h5-7,1
InchiKey:	NYMUOQQNKQPAME-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	279.33

Physical Properties

Property code	Value	Unit	Source
gf	-200.25	kJ/mol	Joback Method
hf	-564.00	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.158		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2354.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	777.01	K	Joback Method
tc	981.78	K	Joback Method
tf	494.73	K	Joback Method
vc	0.851	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.74	J/mol×K	777.01	Joback Method
cpg	662.86	J/mol×K	811.14	Joback Method
cpg	676.00	J/mol×K	845.27	Joback Method
cpg	688.16	J/mol×K	879.40	Joback Method
cpg	699.37	J/mol×K	913.52	Joback Method
cpg	709.63	J/mol×K	947.65	Joback Method
cpg	718.96	J/mol×K	981.78	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=U321706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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