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

Inchi: InChI=1S/C15H21NO4/c1-11(2)10-20-14(17)7-8-16-15(18)12-5-4-6-13(9-12)19-3/h4-6,9,
InchiKey: MIGNQEYWFONBNO-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: COc1cccc(C(=O)NCCC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-202.69	kJ/mol	Joback Method
hf	-569.28	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.014		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	776.57	K	Joback Method
tc	984.18	K	Joback Method
tf	479.73	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/mol×K	776.57	Joback Method
cpg	663.62	J/mol×K	811.17	Joback Method
cpg	676.92	J/mol×K	845.77	Joback Method
cpg	689.21	J/mol×K	880.38	Joback Method
cpg	700.50	J/mol×K	914.98	Joback Method
cpg	710.81	J/mol×K	949.58	Joback Method
cpg	720.14	J/mol×K	984.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321705&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

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