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

Inchi: InChI=1S/C15H21NO3/c1-11(2)10-19-14(17)7-8-16-15(18)13-6-4-5-12(3)9-13/h4-6,9,11H

InchiKey: FOUDYOJQINQPBV-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: Cc1cccc(C(=O)NCCC(=O)OCC(C)C)c1

Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-97.69	kJ/mol	Joback Method
hf	-437.06	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	73.87	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.314		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2156.00		NIST Webbook
tb	754.15	K	Joback Method
tc	962.94	K	Joback Method
tf	457.50	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.01	J/mol×K	754.15	Joback Method
cpg	636.72	J/mol×K	788.95	Joback Method
cpg	650.44	J/mol×K	823.75	Joback Method
cpg	663.19	J/mol×K	858.55	Joback Method
cpg	675.00	J/mol×K	893.35	Joback Method
cpg	685.89	J/mol×K	928.15	Joback Method
cpg	695.89	J/mol×K	962.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321626&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