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

Inchi: InChI=1S/C17H25NO3/c1-13(2)6-5-11-21-16(19)9-10-18-17(20)15-8-4-7-14(3)12-15/h4,7

InchiKey: FFFIGCZGYBFMAM-UHFFFAOYSA-N

Formula: C17H25NO3

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

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-80.85	kJ/mol	Joback Method
hf	-478.34	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.094		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	799.91	K	Joback Method
tc	1005.41	K	Joback Method
tf	480.04	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.88	J/mol×K	799.91	Joback Method
cpg	749.14	J/mol×K	834.16	Joback Method
cpg	763.35	J/mol×K	868.41	Joback Method
cpg	776.54	J/mol×K	902.66	Joback Method
cpg	788.75	J/mol×K	936.91	Joback Method
cpg	800.01	J/mol×K	971.16	Joback Method
cpg	810.35	J/mol×K	1005.41	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=U321628&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