«beta»-Alanine, N-(4-ethylbenzoyl)-, isohexyl ester

Inchi: InChI=1S/C18H27NO3/c1-4-15-7-9-16(10-8-15)18(21)19-12-11-17(20)22-13-5-6-14(2)3/h

InchiKey: MCFDIPXWAVUTGP-UHFFFAOYSA-N

Formula: C18H27NO3

SMILES: CCc1ccc(C(=O)NCCC(=O)OCCCC(C)C)cc1

Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-72.43	kJ/mol	Joback Method
hf	-498.98	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.348		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	822.79	K	Joback Method
tc	1027.52	K	Joback Method
tf	491.31	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.25	J/mol×K	822.79	Joback Method
cpg	806.73	J/mol×K	856.91	Joback Method
cpg	821.14	J/mol×K	891.03	Joback Method
cpg	834.52	J/mol×K	925.15	Joback Method
cpg	846.88	J/mol×K	959.28	Joback Method
cpg	858.27	J/mol×K	993.40	Joback Method
cpg	868.72	J/mol×K	1027.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321654&Units=SI

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