«beta»-Alanine, N-(2-methylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C16H23NO3/c1-3-4-7-12-20-15(18)10-11-17-16(19)14-9-6-5-8-13(14)2/h5-6,8-

InchiKey: LSSOGFZSYDGALG-UHFFFAOYSA-N

Formula: C16H23NO3

SMILES: CCCCCOC(=O)CCNC(=O)c1ccccc1C

Mol. weight [g/mol]: 277.36

Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-452.42	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	2.848		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2248.00		NIST Webbook
tb	777.47	K	Joback Method
tc	981.54	K	Joback Method
tf	483.77	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/mol×K	777.47	Joback Method
cpg	691.69	J/mol×K	811.48	Joback Method
cpg	705.50	J/mol×K	845.49	Joback Method
cpg	718.36	J/mol×K	879.50	Joback Method
cpg	730.30	J/mol×K	913.51	Joback Method
cpg	741.33	J/mol×K	947.53	Joback Method
cpg	751.49	J/mol×K	981.54	Joback Method

Sources

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=U321615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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