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

Inchi: InChI=1S/C14H19NO3/c1-3-10-18-13(16)8-9-15-14(17)12-7-5-4-6-11(12)2/h4-7H,3,8-10

InchiKey: WRZIYDBAFRCQKF-UHFFFAOYSA-N

Formula: C14H19NO3

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

Mol. weight [g/mol]: 249.31

Physical Properties

Property code	Value	Unit	Source
gf	-103.67	kJ/mol	Joback Method
hf	-411.14	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.068		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	731.71	K	Joback Method
tc	939.56	K	Joback Method
tf	461.23	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.10	J/mol×K	731.71	Joback Method
cpg	581.23	J/mol×K	766.35	Joback Method
cpg	594.43	J/mol×K	800.99	Joback Method
cpg	606.73	J/mol×K	835.63	Joback Method
cpg	618.15	J/mol×K	870.28	Joback Method
cpg	628.71	J/mol×K	904.92	Joback Method
cpg	638.43	J/mol×K	939.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321613&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