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

Inchi: InChI=1S/C13H17NO3/c1-3-17-12(15)8-9-14-13(16)11-7-5-4-6-10(11)2/h4-7H,3,8-9H2,1

InchiKey: LFIWGGFBHZLOHV-UHFFFAOYSA-N

Formula: C13H17NO3

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

Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-112.09	kJ/mol	Joback Method
hf	-390.50	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.678		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	708.83	K	Joback Method
tc	919.30	K	Joback Method
tf	449.96	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.91	J/mol×K	708.83	Joback Method
cpg	527.62	J/mol×K	743.91	Joback Method
cpg	540.44	J/mol×K	778.99	Joback Method
cpg	552.38	J/mol×K	814.07	Joback Method
cpg	563.47	J/mol×K	849.14	Joback Method
cpg	573.71	J/mol×K	884.22	Joback Method
cpg	583.15	J/mol×K	919.30	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=U321612&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