.BETA.-alanine, n-(4-methylbenzoyl)-, ethyl ester

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

InchiKey: SSXFUIIOIDYWMG-UHFFFAOYSA-N

Formula: C13H17NO3

SMILES: CCOC(=O)CCNC(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
af	0.7090		Cheméo Relay (1.0)
hf	-536.43	kJ/mol	Cheméo Relay (1.0)
hfus	32.56	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-2.88		Cheméo Relay (1.0)
logp	1.678		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	2029.00		NIST Webbook
tb	606.20	K	Cheméo Relay (1.0)
tc	814.37	K	Cheméo Relay (1.0)
tf	350.66	K	Cheméo Relay (1.0)
vc	0.689	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321599&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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