.BETA.-alanine, n-(4-ethylbenzoyl)-, propyl ester

Inchi: InChI=1S/C15H21NO3/c1-3-11-19-14(17)9-10-16-15(18)13-7-5-12(4-2)6-8-13/h5-8H,3-4

InchiKey: RLSLIEFJHUWGFC-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: CCCOC(=O)CCNC(=O)c1ccc(CC)cc1

Mol. weight [g/mol]: 263.34

Physical Properties

Property code	Value	Unit	Source
hf	-568.21	kJ/mol	Cheméo Relay (1.0)
hfus	37.74	kJ/mol	Joback Method
hvap	93.63	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.53		Cheméo Relay (1.0)
logp	2.322		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2225.00		NIST Webbook
tb	616.61	K	Cheméo Relay (1.0)
tc	831.50	K	Cheméo Relay (1.0)
tf	312.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.45	J/mol×K	754.59	Joback Method
cpg	635.94	J/mol×K	788.87	Joback Method
cpg	649.47	J/mol×K	823.16	Joback Method
cpg	662.07	J/mol×K	857.44	Joback Method
cpg	673.77	J/mol×K	891.72	Joback Method
cpg	684.59	J/mol×K	926.01	Joback Method
cpg	694.55	J/mol×K	960.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321651&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):	
Cheméo Relay (1.0, beta):	

Legend

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
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