

«beta»- Alanine, N-(3-methylbenzoyl)-, ethyl ester

Inchi:	InChI=1S/C13H17NO3/c1-3-17-12(15)7-8-14-13(16)11-6-4-5-10(2)9-11/h4-6,9H,3,7-8H2
InchiKey:	XGJJYYYYJPAKHJA-UHFFFAOYSA-N
Formula:	C13H17NO3
SMILES:	CCOC(=O)CCNC(=O)c1cccc(C)c1
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
rinpola	2008.00		NIST Webbook
rinpola	2008.00		NIST Webbook
tb	708.83	K	Joback Method
tc	919.30	K	Joback Method
tf	449.96	K	Joback Method
vc	0.721	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

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=U321625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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