

Glycine, N-(4-methylbenzoyl)-, methyl ester

Other names:	Glycine, N-(p-toluoyl)-, methyl ester
Inchi:	InChI=1S/C11H13NO3/c1-8-3-5-9(6-4-8)11(14)12-7-10(13)15-2/h3-6H,7H2,1-2H3,(H,12,
InchiKey:	OIBNTNKRKWKBQG-UHFFFAOYSA-N
Formula:	C11H13NO3
SMILES:	COC(=O)CNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	207.23
CAS:	1208-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-349.22	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	0.898		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook
tb	663.07	K	Joback Method
tc	880.04	K	Joback Method
tf	427.42	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.36	J/molxK	663.07	Joback Method
cpg	424.02	J/molxK	699.23	Joback Method
cpg	435.84	J/molxK	735.39	Joback Method
cpg	446.86	J/molxK	771.56	Joback Method
cpg	457.08	J/molxK	807.72	Joback Method
cpg	466.52	J/molxK	843.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C1208237&Units=SI

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

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