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

Physical Properties

Property code	Value	Unit	Source
hf	-468.26	kJ/mol	Cheméo Relay (1.0)
hfus	27.38	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-2.63		Cheméo Relay (1.0)
logp	0.898		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
rinpol	1781.00		NIST Webbook
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tb	583.17	K	Cheméo Relay (1.0)
tc	797.73	K	Cheméo Relay (1.0)
tf	370.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.36	J/mol×K	663.07	Joback Method
cpg	424.02	J/mol×K	699.23	Joback Method
cpg	435.84	J/mol×K	735.39	Joback Method
cpg	446.86	J/mol×K	771.56	Joback Method
cpg	457.08	J/mol×K	807.72	Joback Method
cpg	466.52	J/mol×K	843.88	Joback Method
cpg	475.19	J/mol×K	880.04	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1208237&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point