Hippuric acid, methyl ester

Other names:	Glycine, N-benzoyl-, methyl ester
	Methyl hippurate
	Methyl N-benzoylglycinate
	N-Benzoylglycine methyl ester
	Methyl ester of hippuric acid
	Methyl (benzoylamino)acetate
	Benzoylamino-acetic acid methyl ester
Inchi:	InChI=1S/C10H11NO3/c1-14-9(12)7-11-10(13)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,11,13)
InchiKey:	XTKVNQKOTKPCKM-UHFFFAOYSA-N
Formula:	C10H11NO3
SMILES:	COC(=O)CNC(=O)c1ccccc1
Mol. weight [g/mol]:	193.20
CAS:	1205-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-127.72	kJ/mol	Joback Method
hf	-317.11	kJ/mol	Joback Method
hfus	25.18	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	0.589		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1715.40		NIST Webbook
rinpol	1720.80		NIST Webbook
rinpol	1722.20		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	635.21	K	Joback Method
tc	855.07	K	Joback Method
tf	403.63	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.30	J/mol×K	635.21	Joback Method
cpg	375.49	J/mol×K	671.85	Joback Method
cpg	386.85	J/mol×K	708.50	Joback Method
cpg	397.40	J/mol×K	745.14	Joback Method
cpg	407.16	J/mol×K	781.78	Joback Method
cpg	416.15	J/mol×K	818.42	Joback Method
cpg	424.40	J/mol×K	855.07	Joback Method

Sources

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=C1205089&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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