Glycine, N-(2-hydroxybenzoyl)-, methyl ester

Other names:	Methyl o-hydroxyhippurate
	o-Hydroxyhippuric acid methyl ester
	o-Hydroxyhippuric , methyl ester
	Methyl salicylurate
Inchi:	InChI=1S/C10H11NO4/c1-15-9(13)6-11-10(14)7-4-2-3-5-8(7)12/h2-5,12H,6H2,1H3,(H,11
InchiKey:	PXFSDQXXIDCRPA-UHFFFAOYSA-N
Formula:	C10H11NO4
SMILES:	COC(=O)CNC(=O)c1ccccc1O
Mol. weight [g/mol]:	209.20
CAS:	55493-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-282.34	kJ/mol	Joback Method
hf	-494.42	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.295		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1750.00		NIST Webbook
tb	715.83	K	Joback Method
tc	943.94	K	Joback Method
tf	515.35	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.23	J/mol×K	715.83	Joback Method
cpg	418.75	J/mol×K	753.85	Joback Method
cpg	428.55	J/mol×K	791.87	Joback Method
cpg	437.71	J/mol×K	829.89	Joback Method

cpg	446.29	J/mol×K	867.91	Joback Method
cpg	454.36	J/mol×K	905.93	Joback Method
cpg	461.98	J/mol×K	943.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55493895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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