

Hippuric acid, p-chloro-

Inchi:	InChI=1S/C9H8ClNO3/c10-7-3-1-6(2-4-7)9(14)11-5-8(12)13/h1-4H,5H2,(H,11,14)(H,12,13)
InchiKey:	COYZIYOEXGRBHQ-UHFFFAOYSA-N
Formula:	C9H8ClNO3
SMILES:	O=C(O)CNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	213.62
CAS:	13450-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-189.52	kJ/mol	Joback Method
hf	-343.69	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.154		Crippen Method
mcvol	145.140	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	724.50	K	Joback Method
tc	938.69	K	Joback Method
tf	473.39	K	Joback Method
vc	0.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.65	J/mol×K	724.50	Joback Method
cpg	363.83	J/mol×K	760.20	Joback Method
cpg	371.38	J/mol×K	795.90	Joback Method
cpg	378.33	J/mol×K	831.60	Joback Method
cpg	384.72	J/mol×K	867.29	Joback Method
cpg	390.56	J/mol×K	902.99	Joback Method
cpg	395.90	J/mol×K	938.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13450776&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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