

Hippuric acid di-methyl derivative

Other names:	Hippuric acid di-methyl derivative
Inchi:	InChI=1S/C11H13NO3/c1-12(8-10(13)15-2)11(14)9-6-4-3-5-7-9/h3-7H,8H2,1-2H3
InchiKey:	VJKASHDUZIYFTQ-UHFFFAOYSA-N
Formula:	C11H13NO3
SMILES:	COC(=O)CN(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	207.23

Physical Properties

Property code	Value	Unit	Source
af	0.5802		Cheméo Relay (1.0)
hf	-398.06	kJ/mol	Cheméo Relay (1.0)
hfus	25.69	kJ/mol	Joback Method
hvap	81.59	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-1.70		Cheméo Relay (1.0)
logp	0.932		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	576.28	K	Cheméo Relay (1.0)
tc	771.35	K	Cheméo Relay (1.0)
tf	302.22	K	Cheméo Relay (1.0)
vc	0.587	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.97	J/mol×K	620.36	Joback Method
cpg	413.56	J/mol×K	655.99	Joback Method
cpg	426.24	J/mol×K	691.63	Joback Method
cpg	438.06	J/mol×K	727.26	Joback Method
cpg	449.03	J/mol×K	762.90	Joback Method
cpg	459.20	J/mol×K	798.53	Joback Method
cpg	468.58	J/mol×K	834.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C71533216&Units=SI

Legend

af:	Acentric Factor
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
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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