Homovanillic acid

Other names:	Benzeneacetic acid, 4-hydroxy-3-methoxy- Acetic acid, (4-hydroxy-3-methoxyphenyl)- (4-Hydroxy-3-methoxyphenyl)acetic acid HMPA HVA Vanillacetic Acid 3-Methoxy-4-hydroxyphenylacetic acid 4-Hydroxy-3-methoxybenzeneacetic acid Homovanillinic acid Homovanilic acid Vanilacetic acid NSC 16682
Inchi:	InChI=1S/C9H10O4/c1-13-8-4-6(5-9(11)12)2-3-7(8)10/h2-4,10H,5H2,1H3,(H,11,12)
InchiKey:	QRMZSPFSDQBLIX-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COc1cc(CC(=O)O)ccc1O
Mol. weight [g/mol]:	182.17
CAS:	306-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-397.68	kJ/mol	Joback Method
hf	-578.37	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.028		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1685.00		NIST Webbook
ripol	3099.00		NIST Webbook
ripol	3099.00		NIST Webbook
ripol	3099.00		NIST Webbook

tb	686.07	K	Joback Method
tc	897.62	K	Joback Method
tf	474.83	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.80	J/mol×K	686.07	Joback Method
cpg	385.63	J/mol×K	862.36	Joback Method
cpg	378.51	J/mol×K	827.10	Joback Method
cpg	371.01	J/mol×K	791.85	Joback Method
cpg	363.09	J/mol×K	756.59	Joback Method
cpg	354.70	J/mol×K	721.33	Joback Method
cpg	392.42	J/mol×K	897.62	Joback Method
dvisc	0.0000060	Pa×s	686.07	Joback Method
dvisc	0.0000094	Pa×s	650.86	Joback Method
dvisc	0.0000156	Pa×s	615.66	Joback Method
dvisc	0.0000275	Pa×s	580.45	Joback Method
dvisc	0.0000520	Pa×s	545.24	Joback Method
dvisc	0.0001077	Pa×s	510.04	Joback Method
dvisc	0.0002480	Pa×s	474.83	Joback Method

Sources

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=C306081&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume