Benzeneacetic acid, 4-hydroxy-

Other names:	(4-Hydroxyphenyl)acetic acid
	(p-Hydroxyphenyl)acetic acid
	4-Hydroxybenzeneacetic acid
	4-hydroxyphenylacetic acid
	Acetic acid, (p-hydroxyphenyl)-
	Parahydroxy phenylacetic acid
Inchi:	InChI=1S/C8H8O3/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4,9H,5H2,(H,10,11)
InchiKey:	XQXPVVBIMDBYFF-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	O=C(O)Cc1ccc(O)cc1
Mol. weight [g/mol]:	152.15
CAS:	156-38-7

Physical Properties

Property code	Value	Unit	Source
gf	-291.47	kJ/mol	Joback Method
hf	-414.04	kJ/mol	Joback Method
hfus	21.99	kJ/mol	Joback Method
hvap	72.12	kJ/mol	Joback Method
ie	8.12 ± 0.02	eV	NIST Webbook
log10ws	-0.94		Aqueous Solubility Prediction Method
logp	1.019		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
rinpol	1557.80		NIST Webbook
rinpol	1545.00		NIST Webbook
tb	635.79	K	Joback Method
tc	852.27	K	Joback Method
tf	423.60 ± 0.50	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	314.43	J/mol×K	816.19	Joback Method
cpg	308.07	J/mol×K	780.11	Joback Method
cpg	301.35	J/mol×K	744.03	Joback Method
cpg	294.18	J/mol×K	707.95	Joback Method
cpg	286.52	J/mol×K	671.87	Joback Method
cpg	278.28	J/mol×K	635.79	Joback Method
cpg	320.49	J/mol×K	852.27	Joback Method
dvisc	0.0008431	Pa×s	428.81	Joback Method
dvisc	0.0000122	Pa×s	635.79	Joback Method
dvisc	0.0000202	Pa×s	601.29	Joback Method
dvisc	0.0000356	Pa×s	566.80	Joback Method
dvisc	0.0000673	Pa×s	532.30	Joback Method
dvisc	0.0001391	Pa×s	497.80	Joback Method
dvisc	0.0003202	Pa×s	463.31	Joback Method
hfust	28.00	kJ/mol	422.90	NIST Webbook
hfust	28.40	kJ/mol	423.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C156387&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfust: Enthalpy of fusion at a given temperature
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