

Benzeneacetic acid, 2-hydroxy-

Other names:	Acetic acid, (o-hydroxyphenyl)- (o-Hydroxyphenyl)acetic acid (2-Hydroxyphenyl)acetic acid 2-Hydroxybenzeneacetic acid ortho-Hydroxyphenylacetic acid
Inchi:	InChI=1S/C8H8O3/c9-7-4-2-1-3-6(7)5-8(10)11/h1-4,9H,5H2,(H,10,11)
InchiKey:	CCVYRRGZDBSHFU-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	O=C(O)Cc1ccccc1O
Mol. weight [g/mol]:	152.15
CAS:	614-75-5

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	8.16 ± 0.02	eV	NIST Webbook
log10ws	-0.92		Crippen Method
logp	1.019		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
tb	635.79	K	Joback Method
tc	852.27	K	Joback Method
tf	420.00 ± 2.00	K	NIST Webbook
tf	422.00 ± 3.00	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.28	J/molxK	635.79	Joback Method
cpg	286.52	J/molxK	671.87	Joback Method

cpg	294.18	J/mol×K	707.95	Joback Method
cpg	301.35	J/mol×K	744.03	Joback Method
cpg	308.07	J/mol×K	780.11	Joback Method
cpg	314.43	J/mol×K	816.19	Joback Method
cpg	320.49	J/mol×K	852.27	Joback Method
dvisc	0.0008431	Paxs	428.81	Joback Method
dvisc	0.0003202	Paxs	463.31	Joback Method
dvisc	0.0001391	Paxs	497.80	Joback Method
dvisc	0.0000673	Paxs	532.30	Joback Method
dvisc	0.0000356	Paxs	566.80	Joback Method
dvisc	0.0000202	Paxs	601.29	Joback Method
dvisc	0.0000122	Paxs	635.79	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=C614755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
ie:	Ionization energy
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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