

Hydroquinone, acetate

Inchi:

InChI=1S/C8H8O3/c1-6(9)11-8-4-2-7(10)3-5-8/h2-5,10H,1H3

InchiKey:

HBMCQTHGYMTCOF-UHFFFAOYSA-N

Formula:

C8H8O3

SMILES:

CC(=O)Oc1ccc(O)cc1

Mol. weight [g/mol]:

152.15

Physical Properties

Property code	Value	Unit	Source
gf	-259.65	kJ/mol	Joback Method
hf	-394.03	kJ/mol	Joback Method
hfus	19.09	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.317		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
tb	566.03	K	Joback Method
tc	798.25	K	Joback Method
tf	390.22	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.25	J/mol×K	566.03	Joback Method
cpg	269.54	J/mol×K	604.73	Joback Method
cpg	279.09	J/mol×K	643.44	Joback Method
cpg	287.96	J/mol×K	682.14	Joback Method
cpg	296.23	J/mol×K	720.84	Joback Method
cpg	303.95	J/mol×K	759.54	Joback Method
cpg	311.19	J/mol×K	798.25	Joback Method
dvisc	0.0011881	Pa×s	390.22	Joback Method

dvisc	0.0005829	Pa×s	419.52	Joback Method
dvisc	0.0003139	Pa×s	448.82	Joback Method
dvisc	0.0001823	Pa×s	478.12	Joback Method
dvisc	0.0001128	Pa×s	507.43	Joback Method
dvisc	0.0000735	Pa×s	536.73	Joback Method
dvisc	0.0000501	Pa×s	566.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352777&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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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