

Benzeneacetic acid, 4-hydroxy-, methyl ester

Other names:	Acetic acid, (p-hydroxyphenyl)-, methyl ester Methyl (p-hydroxyphenyl)acetate Methyl (4-hydroxyphenyl)acetate 4-Hydroxyphenylacetic acid methyl ester p-Hydroxyphenylacetic acid methyl ester
Inchi:	InChI=1S/C9H10O3/c1-12-9(11)6-7-2-4-8(10)5-3-7/h2-5,10H,6H2,1H3
InchiKey:	XGDZEDRBLVIUMX-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)Cc1ccc(O)cc1
Mol. weight [g/mol]:	166.17
CAS:	14199-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-251.23	kJ/mol	Joback Method
hf	-414.67	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.108		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	588.91	K	Joback Method
tc	816.64	K	Joback Method
tf	401.49	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	304.03	J/molxK	588.91	Joback Method
cpg	353.29	J/molxK	778.68	Joback Method
cpg	344.71	J/molxK	740.73	Joback Method
cpg	335.56	J/molxK	702.77	Joback Method
cpg	325.77	J/molxK	664.82	Joback Method
cpg	315.28	J/molxK	626.86	Joback Method
cpg	361.35	J/molxK	816.64	Joback Method
dvisc	0.0000400	Paxs	588.91	Joback Method
dvisc	0.0000590	Paxs	557.67	Joback Method
dvisc	0.0000909	Paxs	526.44	Joback Method
dvisc	0.0001481	Paxs	495.20	Joback Method
dvisc	0.0002577	Paxs	463.96	Joback Method
dvisc	0.0004856	Paxs	432.73	Joback Method
dvisc	0.0010100	Paxs	401.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.70	K	0.70	NIST Webbook

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=C14199156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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