

Benzenemehanol, 4-hydroxy-3-methoxy, acetate

Inchi:	InChI=1S/C10H12O4/c1-7(11)14-6-8-3-4-9(12)10(5-8)13-2/h3-5,12H,6H2,1-2H3
InchiKey:	DZWDEGBGKYCSKL-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cc(COC(C)=O)ccc1O
Mol. weight [g/mol]:	196.20

Physical Properties

Property code	Value	Unit	Source
gf	-357.44	kJ/mol	Joback Method
hf	-579.00	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.464		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	639.19	K	Joback Method
tc	860.68	K	Joback Method
tf	447.51	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.77	J/molxK	639.19	Joback Method
cpg	384.49	J/molxK	676.10	Joback Method
cpg	395.53	J/molxK	713.02	Joback Method
cpg	405.91	J/molxK	749.93	Joback Method
cpg	415.69	J/molxK	786.85	Joback Method
cpg	424.90	J/molxK	823.76	Joback Method
cpg	433.57	J/molxK	860.68	Joback Method
dvisc	0.0003718	Paxs	447.51	Joback Method
dvisc	0.0001978	Paxs	479.46	Joback Method
dvisc	0.0001139	Paxs	511.40	Joback Method

dvisc	0.0000700	Paxs	543.35	Joback Method
dvisc	0.0000454	Paxs	575.30	Joback Method
dvisc	0.0000308	Paxs	607.24	Joback Method
dvisc	0.0000217	Paxs	639.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R69952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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