

Benzoic acid, 4-hydroxy-3,5-dimethyl-

Inchi:	InChI=1S/C9H10O3/c1-5-3-7(9(11)12)4-6(2)8(5)10/h3-4,10H,1-2H3,(H,11,12)
InchiKey:	OMNHTTWQSSUZHO-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	Cc1cc(C(=O)O)cc(C)c1O
Mol. weight [g/mol]:	166.17
CAS:	4919-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-302.31	kJ/mol	Joback Method
hf	-457.62	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.707		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4583.94	kPa	Joback Method
tb	668.63	K	Joback Method
tc	883.29	K	Joback Method
tf	465.12	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.76	J/molxK	668.63	Joback Method
cpg	330.56	J/molxK	704.41	Joback Method
cpg	338.84	J/molxK	740.18	Joback Method
cpg	346.68	J/molxK	775.96	Joback Method
cpg	354.13	J/molxK	811.74	Joback Method
cpg	361.25	J/molxK	847.51	Joback Method
cpg	368.09	J/molxK	883.29	Joback Method
dvisc	0.0003242	Paxs	465.12	Joback Method
dvisc	0.0001437	Paxs	499.04	Joback Method

dvisc	0.0000706	Paxs	532.96	Joback Method
dvisc	0.0000378	Paxs	566.88	Joback Method
dvisc	0.0000217	Paxs	600.79	Joback Method
dvisc	0.0000132	Paxs	634.71	Joback Method
dvisc	0.0000085	Paxs	668.63	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=C4919373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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