

4-Hydroxy-3-methoxybenzyl alcohol

Other names:	Benzenemethanol, 4-hydroxy-3-methoxy- Vanillic alcohol Vanillin alcohol Vanillol benzyl alcohol, 4-hydroxy-3-methoxy- vanillyl alcohol
Inchi:	InChI=1S/C8H10O3/c1-11-8-4-6(5-9)2-3-7(8)10/h2-4,9-10H,5H2,1H3
InchiKey:	ZENOXNGFMSCLLL-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	<chem>COc1cc(CO)ccc1O</chem>
Mol. weight [g/mol]:	154.16
CAS:	498-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-277.18	kJ/mol	Joback Method
hf	-445.15	kJ/mol	Joback Method
hfus	21.19	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.893		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
ripol	2764.00		NIST Webbook
ripol	2787.00		NIST Webbook
ripol	2787.00		NIST Webbook
ripol	2787.00		NIST Webbook
tb	609.32	K	Joback Method
tc	817.37	K	Joback Method
tf	351.15 ± 1.50	K	NIST Webbook
tf	389.00	K	Solubility and thermodynamic properties of vanillyl alcohol in some pure solvents
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.55	J/molxK	817.37	Joback Method
cpg	298.88	J/molxK	644.00	Joback Method
cpg	307.49	J/molxK	678.67	Joback Method
cpg	315.62	J/molxK	713.35	Joback Method
cpg	323.31	J/molxK	748.02	Joback Method
cpg	330.61	J/molxK	782.70	Joback Method
cpg	289.75	J/molxK	609.32	Joback Method
dvisc	0.0000195	Paxs	576.70	Joback Method
dvisc	0.0000342	Paxs	544.09	Joback Method
dvisc	0.0000644	Paxs	511.47	Joback Method
dvisc	0.0001322	Paxs	478.86	Joback Method
dvisc	0.0003013	Paxs	446.25	Joback Method
dvisc	0.0000118	Paxs	609.32	Joback Method
dvisc	0.0007825	Paxs	413.63	Joback Method
psub	6.50e-04	kPa	346.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	8.15e-04	kPa	348.13	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.06e-03	kPa	350.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.12e-04	kPa	332.19	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.48e-04	kPa	334.36	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol

psub	1.82e-04	kPa	336.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	2.37e-04	kPa	338.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.07e-04	kPa	340.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	5.06e-04	kPa	344.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	5.06e-04	kPa	344.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	6.42e-04	kPa	346.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	8.07e-04	kPa	348.13	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.04e-03	kPa	350.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.10e-04	kPa	332.19	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.41e-04	kPa	334.36	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol

psub	1.76e-04	kPa	336.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	2.34e-04	kPa	338.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	2.98e-04	kPa	340.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.70e-04	kPa	342.14	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	4.94e-04	kPa	344.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	6.23e-04	kPa	346.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	7.74e-04	kPa	348.13	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.01e-03	kPa	350.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.92e-04	kPa	342.14	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.12e-04	kPa	340.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol

psub	2.40e-04	kPa	338.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.87e-04	kPa	336.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.47e-04	kPa	334.36	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.13e-04	kPa	332.19	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.85e-04	kPa	342.14	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C498000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Comprehensive thermophysical and thermochemical studies of vanillyl alcohol	https://www.doi.org/10.1016/j.jct.2016.07.015
Solubility and thermodynamic properties of vanillyl alcohol in some papers	https://www.doi.org/10.1016/j.jct.2016.11.030
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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