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:	COc1cc(CO)ccc1O
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	289.75	J/mol×K	609.32	Joback Method
cpg	298.88	J/mol×K	644.00	Joback Method
cpg	307.49	J/mol×K	678.67	Joback Method
cpg	315.62	J/mol×K	713.35	Joback Method
cpg	323.31	J/mol×K	748.02	Joback Method
cpg	330.61	J/mol×K	782.70	Joback Method
cpg	337.55	J/mol×K	817.37	Joback Method
dvisc	0.0007825	Pa×s	413.63	Joback Method
dvisc	0.0003013	Pa×s	446.25	Joback Method
dvisc	0.0001322	Pa×s	478.86	Joback Method
dvisc	0.0000644	Pa×s	511.47	Joback Method
dvisc	0.0000342	Pa×s	544.09	Joback Method
dvisc	0.0000195	Pa×s	576.70	Joback Method
dvisc	0.0000118	Pa×s	609.32	Joback Method
psub	8.15e-04	kPa	348.13	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.47e-04	kPa	334.36	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.87e-04	kPa	336.15	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	2.40e-04	kPa	338.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	3.12e-04	kPa	340.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol

psub	3.92e-04	kPa	342.14	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	5.06e-04	kPa	344.21	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	6.50e-04	kPa	346.27	Comprehensive thermophysical and thermochemical studies of vanillyl alcohol
psub	1.13e-04	kPa	332.19	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	3.85e-04	kPa	342.14	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

Sources

Solubility and thermodynamic properties of vanillyl alcohol in some pure solvents:	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
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

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

Latest version available from:

https://www.chemeo.com/cid/56-154-9/4-Hydroxy-3-methoxybenzyl-alcohol.pdf

Generated by Cheméo on 2024-10-12 07:57:03.573599007 +0000 UTC m=+3300686.210568255.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.