m-Guaiacol

Other names:	1-Hydroxy-3-methoxybenzene
	3-Hydroxyanisole
	3-methoxyphenol
	NSC 21735
	Phenol, m-methoxy-
	Resorcinol methyl ether
	Resorcinol monomethyl ether
	m-Hydroxyanisol
	m-Hydroxyanisole
	m-methoxyphenol
	phenol, 3-methoxy-
Inchi:	InChI=1S/C7H8O2/c1-9-7-4-2-3-6(8)5-7/h2-5,8H,1H3
InchiKey:	ASHGTJPOSUFTGB-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	COc1cccc(O)c1
Mol. weight [g/mol]:	124.14
CAS:	150-19-6

Physical Properties

Property code	Value	Unit	Source
gf	-139.15	kJ/mol	Joback Method
hf	-260.81	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	75.90 ± 1.20	kJ/mol	NIST Webbook
log10ws	-1.14		Crippen Method
logp	1.401		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1234.80		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1211.00		NIST Webbook
ripol	2086.00		NIST Webbook
tb	517.00	K	NIST Webbook
tc	716.68	K	Joback Method
tf	329.02	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.43	J/mol×K	489.28	Joback Method
cpg	215.86	J/mol×K	527.18	Joback Method
cpg	225.57	J/mol×K	565.08	Joback Method
cpg	234.59	J/mol×K	602.98	Joback Method
cpg	243.00	J/mol×K	640.88	Joback Method
cpg	250.84	J/mol×K	678.78	Joback Method
cpg	258.19	J/mol×K	716.68	Joback Method
dvisc	0.0032569	Pa×s	329.02	Joback Method
dvisc	0.0014199	Pa×s	355.73	Joback Method
dvisc	0.0006951	Pa×s	382.44	Joback Method
dvisc	0.0003736	Pa×s	409.15	Joback Method
dvisc	0.0002167	Pa×s	435.86	Joback Method
dvisc	0.0001338	Pa×s	462.57	Joback Method
dvisc	0.0000871	Pa×s	489.28	Joback Method
hvapt	64.80	kJ/mol	465.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	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=C150196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibrium Measurements for Model Systems Related to Catalytic Fast Pyrolysis of Biomass:	https://www.doi.org/10.1021/acs.jced.6b00625

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	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