Mequinol

Other names:	1-Hydroxy-4-methoxybenzene
	4-Hydroxyanisole
	4-Methoxyphenol
	BMS 181158
	Eastman HQMME
	HQMME
	Hydroquinone methyl ether
	Hydroquinone monomethyl ether
	Hydroxyanisole
	Leucobasal
	Leucodine B
	MEHQ
	MME
	Mechinolum
	Mequinol (INN)
	Monomethyl ether hydroquinone
	NSC 4960
	Novo-dermoquinona
	PMF (antioxidant)
	Phenol, 4-methoxy-
	Phenol, p-methoxy-
	Po-hydroxyanisole
	USAF AN-7
	p-Guaiacol
	p-Hydroxyanisole
	p-Hydroxymethoxybenzene
	p-Methoxyphenol
Inchi:	InChI=1S/C7H8O2/c1-9-7-4-2-6(8)3-5-7/h2-5,8H,1H3
InchiKey:	NWVVVBRKAWDGAB-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	COc1ccc(O)cc1
Mol. weight [g/mol]:	124.14
CAS:	150-76-5

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
hsub	94.40 ± 1.20	kJ/mol	NIST Webbook
hvap	48.88	kJ/mol	Joback Method
ie	8.00 ± 0.10	eV	NIST Webbook
ie	7.50	eV	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	1210.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1234.70		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1197.00		NIST Webbook
tb	516.20	K	NIST Webbook
tb	516.00	K	NIST Webbook
tc	716.68	K	Joback Method
tf	330.15	K	Liquid pharmaceuticals formulation by eutectic formation
tf	326.00	K	NIST Webbook
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.19	J/mol×K	716.68	Joback Method
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
dvisc	0.0000871	Pa×s	489.28	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
hfust	18.30	kJ/mol	328.40	NIST Webbook
hfust	18.30	kJ/mol	328.40	NIST Webbook
hsubt	88.70	kJ/mol	289.00	NIST Webbook
hvapt	61.40	kJ/mol	468.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.36648e+01
Coeff. B	-7.25022e+03
Coeff. C	-8.34070e+01
Temperature range (K), min.	393.55
Temperature range (K), max.	478.44

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150765&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Liquid-Liquid Equilibrium Measurements for Model Systems Related to Catalytic Fast Pyrolysis of Biomass:	https://www.doi.org/10.1021/acs.jced.6b00625
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume