

Creosol

Other names:	Phenol, 2-methoxy-4-methyl- p-Cresol, 2-methoxy- p-Cresol p-Methylguaiacol Homoguaiacol 2-Methoxy-p-cresol 2-Methoxy-4-cresol 2-Methoxy-4-methylphenol 3-Methoxy-4-hydroxytoluene 4-Hydroxy-3-methoxytoluene 4-Methyl-2-methoxyphenol 4-Methylguaiacol 4-Hydroxy-3-methoxy-1-methylbenzene Homocatechol monomethyl ether Valspice Phenol, 4-methyl-2-methoxy NSC 4969 4-Methyl-2-methoxyphenol (4-methylguaiacol) p-methylguaiacol 2-methoxy-4-methylphenol (creosol) 2-Methoxy-4-methylphenol (4-methylguaiacol)
Inchi:	InChI=1S/C8H10O2/c1-6-3-4-7(9)8(5-6)10-2/h3-5,9H,1-2H3
InchiKey:	PETRWTHZSKVLR-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	<chem>COc1cc(C)ccc1O</chem>
Mol. weight [g/mol]:	138.16
CAS:	93-51-6

Physical Properties

Property code	Value	Unit	Source
chl	-4214.40 ± 2.10	kJ/mol	NIST Webbook
gf	-140.36	kJ/mol	Joback Method
hf	-291.90	kJ/mol	NIST Webbook
hfl	-362.80 ± 2.20	kJ/mol	NIST Webbook
hfus	17.10	kJ/mol	Joback Method
hvap	70.90	kJ/mol	NIST Webbook

log10ws	-1.62		Crippen Method
logp	1.709		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
rinpol	1155.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1195.50		NIST Webbook
rinpol	1192.60		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1192.00		NIST Webbook

ripol	1162.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1972.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1972.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1952.00		NIST Webbook
ripol	1946.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1937.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1982.00		NIST Webbook
ripol	1965.00		NIST Webbook
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ripol	1968.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1938.00		NIST Webbook
ripol	1945.00		NIST Webbook
tb	494.20	K	NIST Webbook
tc	741.86	K	Joback Method
tf	352.81	K	Joback Method
vc	0.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.51	J/molxK	517.14	Joback Method
cpg	296.00	J/molxK	704.40	Joback Method
cpg	287.30	J/molxK	666.95	Joback Method
cpg	278.05	J/molxK	629.50	Joback Method
cpg	268.21	J/molxK	592.05	Joback Method
cpg	257.71	J/molxK	554.59	Joback Method
cpg	304.20	J/molxK	741.86	Joback Method
dvisc	0.0000635	Paxs	517.14	Joback Method
dvisc	0.0000946	Paxs	489.75	Joback Method
dvisc	0.0001476	Paxs	462.36	Joback Method
dvisc	0.0002437	Paxs	434.98	Joback Method
dvisc	0.0004303	Paxs	407.59	Joback Method
dvisc	0.0008248	Paxs	380.20	Joback Method
dvisc	0.0017487	Paxs	352.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.70	K	2.90	NIST Webbook
tbrp	384.00 ± 1.00	K	2.00	NIST Webbook

Sources

- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C93516&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
- Joback Method:** https://en.wikipedia.org/wiki/Joback_method
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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

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