2-Methoxy-5-methylphenol

Other names: Phenol, 2-methoxy-5-methyl-
m-Cresol, 6-methoxy-
Isocreosol
5-Methylguaiacol
6-methoxy-m-cresol
Inchi: InChI=1S/C8H10O2/c1-6-3-4-8(10-2)7(9)5-6/h3-5,9H,1-2H3
InchiKey: IFNDEOYXGHGERA-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1ccc(C)cc1O
Mol. weight [g/mol]: 138.16
CAS: 1195-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-140.36	kJ/mol	Joback Method
hf	-292.92	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.709		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
rinpol	1177.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1201.70		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	495.65 ± 1.00	K	NIST Webbook
tc	741.86	K	Joback Method
tf	311.15 ± 0.50	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.00 ± 1.00	K	2.70	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=C1195091&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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