PHENOL, 4-METHOXY-3-METHYL-

Other names: 4-Methoxy-3-methylphenol
Inchi: InChI=1S/C8H10O2/c1-6-5-7(9)3-4-8(6)10-2/h3-5,9H,1-2H3
InchiKey: ILASIIGKRFKNQC-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1ccc(O)cc1C
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
hf	-266.54	kJ/mol	Cheméo Relay (1.0)
hfus	17.10	kJ/mol	Joback Method
hvap	76.37	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-1.17		Cheméo Relay (1.0)
logp	1.709		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
tb	521.79	K	Cheméo Relay (1.0)
tc	727.79	K	Cheméo Relay (1.0)
tf	357.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.51	J/mol×K	517.14	Joback Method
cpg	304.20	J/mol×K	741.86	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
dvisc	0.0002437	Pa×s	434.98	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	0.0017487	Pa×s	352.81	Joback Method
dvisc	0.0004303	Pa×s	407.59	Joback Method
dvisc	0.0008248	Pa×s	380.20	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14786824&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point