3-Methoxy-5-methylphenol

Other names: Phenol, 3-methoxy-5-methyl-
Inchi: InChI=1S/C8H10O2/c1-6-3-7(9)5-8(4-6)10-2/h3-5,9H,1-2H3
InchiKey: NOTCZLKDULMKBR-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1cc(C)cc(O)c1
Mol. weight [g/mol]: 138.16
CAS: 3209-13-0

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	1342.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1342.00		NIST Webbook
ripol	2524.00		NIST Webbook
ripol	2535.00		NIST Webbook
ripol	2535.00		NIST Webbook
tb	517.14	K	Joback Method
tc	741.86	K	Joback Method
tf	352.81	K	Joback Method
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

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=C3209130&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
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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