PHENOL, 2-METHOXY-3-METHYL-

Other names: 2-Methoxy-3-methylphenol
2-Methoxy-2-methyl Phenol
Inchi: InChI=1S/C8H10O2/c1-6-4-3-5-7(9)8(6)10-2/h3-5,9H,1-2H3
InchiKey: SHESIBIEPSTHMZ-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: COc1c(C)cccc1O
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
af	0.5677		Cheméo Relay (1.0)
gf	-140.36	kJ/mol	Joback Method
hf	-264.49	kJ/mol	Cheméo Relay (1.0)
hfus	17.10	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.20		Cheméo Relay (1.0)
logp	1.709		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
ripol	2021.00		NIST Webbook
ripol	2021.00		NIST Webbook
tb	490.05	K	Cheméo Relay (1.0)
tc	721.88	K	Cheméo Relay (1.0)
tf	287.80	K	Cheméo Relay (1.0)
vc	0.390	m3/kmol	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	257.71	J/mol×K	554.59	Joback Method
cpg	268.21	J/mol×K	592.05	Joback Method
cpg	278.05	J/mol×K	629.50	Joback Method

cpg	287.30	J/mol×K	666.95	Joback Method
cpg	296.00	J/mol×K	704.40	Joback Method
cpg	304.20	J/mol×K	741.86	Joback Method
dvisc	0.0017487	Pa×s	352.81	Joback Method
dvisc	0.0008248	Pa×s	380.20	Joback Method
dvisc	0.0004303	Pa×s	407.59	Joback Method
dvisc	0.0002437	Pa×s	434.98	Joback Method
dvisc	0.0001476	Pa×s	462.36	Joback Method
dvisc	0.0000946	Pa×s	489.75	Joback Method
dvisc	0.0000635	Pa×s	517.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18102313&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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