

Phenol, 5-methoxy-2,3,4-trimethyl-

Other names:	3-Methoxy-4,5,6-trimethylphenol 5-Methoxy-2,3,4-trimethylphenol
Inchi:	InChI=1S/C10H14O2/c1-6-7(2)9(11)5-10(12-4)8(6)3/h5,11H,1-4H3
InchiKey:	LFUKZFMVMPZVLII-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	COc1cc(O)c(C)c(C)c1C
Mol. weight [g/mol]:	166.22
CAS:	34883-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-142.78	kJ/mol	Joback Method
hf	-357.14	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Joback Method
hvap	57.54	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.326		Crippen Method
mvol	139.740	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
ripol	2382.00		NIST Webbook
ripol	2382.00		NIST Webbook
tb	572.86	K	Joback Method
tc	791.88	K	Joback Method
tf	400.39	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.80	J/mol×K	572.86	Joback Method
cpg	346.41	J/mol×K	609.36	Joback Method
cpg	358.37	J/mol×K	645.87	Joback Method
cpg	369.71	J/mol×K	682.37	Joback Method
cpg	380.48	J/mol×K	718.88	Joback Method

cpg	390.71	J/molxK	755.38	Joback Method
cpg	400.45	J/molxK	791.88	Joback Method
dvisc	0.0006116	Paxs	400.39	Joback Method
dvisc	0.0003257	Paxs	429.13	Joback Method
dvisc	0.0001877	Paxs	457.88	Joback Method
dvisc	0.0001155	Paxs	486.62	Joback Method
dvisc	0.0000750	Paxs	515.37	Joback Method
dvisc	0.0000510	Paxs	544.12	Joback Method
dvisc	0.0000360	Paxs	572.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34883028&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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