Phenol, 3,4-dimethoxy-

Other names: 3,4-Dimethoxyphenol
Inchi: InChI=1S/C8H10O3/c1-10-7-4-3-6(9)5-8(7)11-2/h3-5,9H,1-2H3
InchiKey: SMFFZOQLHYIRDA-UHFFFAOYSA-N
Formula: C8H10O3
SMILES: COc1ccc(O)cc1OC
Mol. weight [g/mol]: 154.16
CAS: 2033-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-245.36	kJ/mol	Joback Method
hf	-425.14	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.409		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1383.00		NIST Webbook
ripol	2750.00		NIST Webbook
ripol	2738.00		NIST Webbook
ripol	2732.00		NIST Webbook
ripol	2738.00		NIST Webbook
ripol	2750.00		NIST Webbook
tb	539.56	K	Joback Method
tc	761.62	K	Joback Method
tf	375.04	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.41	J/mol×K	539.56	Joback Method

cpg	317.62	J/mol×K	724.61	Joback Method
cpg	308.87	J/mol×K	687.60	Joback Method
cpg	299.60	J/mol×K	650.59	Joback Method
cpg	289.80	J/mol×K	613.58	Joback Method
cpg	279.41	J/mol×K	576.57	Joback Method
cpg	325.89	J/mol×K	761.62	Joback Method
dvisc	0.0000450	Pa×s	539.56	Joback Method
dvisc	0.0000656	Pa×s	512.14	Joback Method
dvisc	0.0000998	Pa×s	484.72	Joback Method
dvisc	0.0001597	Pa×s	457.30	Joback Method
dvisc	0.0002715	Pa×s	429.88	Joback Method
dvisc	0.0004960	Pa×s	402.46	Joback Method
dvisc	0.0009897	Pa×s	375.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2033898&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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