Phenol, 3,4,5-trimethoxy-

Other names:	3,4,5-Trimethoxyphenol
	Antiarol
Inchi:	InChI=1S/C9H12O4/c1-11-7-4-6(10)5-8(12-2)9(7)13-3/h4-5,10H,1-3H3
InchiKey:	VTCDZPUMZAZMSB-UHFFFAOYSA-N
Formula:	C9H12O4
SMILES:	COc1cc(O)cc(OC)c1OC
Mol. weight [g/mol]:	184.19
CAS:	642-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-351.57	kJ/mol	Joback Method
hf	-589.47	kJ/mol	Joback Method
hfus	31.94	kJ/mol	3,4,5-Trimethoxyphenol: A combined experimental and theoretical thermochemical investigation of its antioxidant capacity
hvap	59.47	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.418		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1614.00		NIST Webbook
ripol	3026.00		NIST Webbook
ripol	3065.00		NIST Webbook
ripol	3060.00		NIST Webbook
ripol	3060.00		NIST Webbook
ripol	3049.00		NIST Webbook
ripol	3044.00		NIST Webbook
ripol	3049.00		NIST Webbook
ripol	3060.00		NIST Webbook
tb	589.84	K	Joback Method
tc	806.43	K	Joback Method
tf	421.06	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.73	J/mol×K	806.43	Joback Method
cpg	334.87	J/mol×K	589.84	Joback Method
cpg	346.51	J/mol×K	625.94	Joback Method
cpg	357.61	J/mol×K	662.04	Joback Method
cpg	368.17	J/mol×K	698.13	Joback Method
cpg	378.20	J/mol×K	734.23	Joback Method
cpg	387.72	J/mol×K	770.33	Joback Method
dvisc	0.0000238	Pa×s	589.84	Joback Method
dvisc	0.0003535	Pa×s	421.06	Joback Method
dvisc	0.0001959	Pa×s	449.19	Joback Method
dvisc	0.0001164	Pa×s	477.32	Joback Method
dvisc	0.0000733	Pa×s	505.45	Joback Method
dvisc	0.0000485	Pa×s	533.58	Joback Method
dvisc	0.0000334	Pa×s	561.71	Joback Method
hfust	31.94	kJ/mol	420.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C642717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
3,4,5-Trimethoxyphenol: A combined experimental and theoretical thermochemical investigation of its antioxidant capacity:	https://www.doi.org/10.1016/j.jct.2007.11.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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