Phenol, 3,5-dimethoxy-

Other names:	Phloroglucinol dimethyl ether
	Taxicatigenin
	1-Hydroxy-3,5-dimethoxybenzene
	3,5-Dimethoxyphenol
Inchi:	InChI=1S/C8H10O3/c1-10-7-3-6(9)4-8(5-7)11-2/h3-5,9H,1-2H3
InchiKey:	XQDNFAMOIPNVES-UHFFFAOYSA-N
Formula:	C8H10O3
SMILES:	COc1cc(O)cc(OC)c1
Mol. weight [g/mol]:	154.16
CAS:	500-99-2

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
hsub	101.10 ± 2.30	kJ/mol	NIST Webbook
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	1531.00		NIST Webbook
rinpol	1472.00		NIST Webbook
ripol	2858.00		NIST Webbook
ripol	2848.00		NIST Webbook
ripol	2848.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	2.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C500992&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

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
hsub:	Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume