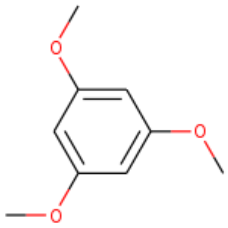
Benzene, 1,3,5-trimethoxy-

Other names: 1,3,5-Trimethoxybenzene; 1,3,5-Trimethyoxybenzene; O,O,O-1,3,5-trimethylresorcinol; Phloroglucinol trimethyl ether.
InChI: InChI=1S/C9H12O3/c1-10-7-4-8(11-2)6-9(5-7)12-3/h4-6H,1-3H3
InChI Key: LKUDPHPHKOZXCD-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: COc1cc(OC)cc(OC)c1
Molecular Weight: 168.19
CAS: 621-23-8



Physical Properties

Property	Value	Unit	Source
PAff	926.70	kJ/mol	NIST Webbook
BasG	898.20	kJ/mol	NIST Webbook
$\Delta_f G°$	-196.95	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-412.16	kJ/mol	Joback Method
$\Delta_{fus} H°$	15.89	kJ/mol	Joback Method
$\Delta_{sub} H°$	100.60 ± 1.90	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	68.20 ± 2.00	kJ/mol	NIST Webbook
IE	7.96	eV	NIST Webbook
$logP_{oct/wat}$	1.712		Crippen Method
P_c	2979.54	kPa	Joback Method
T_{boil}	528.70	K	NIST Webbook
T_c	714.26	K	Joback Method
T_{fus}	309.34	K	Joback Method
V_c	0.485	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	285.91	J/mol×K	509.22	Joback Method
η	0.0001357	Pa×s	509.22	Joback Method
$\Delta_{sub}H$	116.00 ± 1.90	kJ/mol	375.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H12O3/c1-10-7-4-8(11-2)6-9(5-7)12-3/h4-6H,1-3H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

PAff: Proton affinity (kJ/mol).
BasG: Gas basicity (kJ/mol).
$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{sub} H°$: Enthalpy of sublimation at standard conditions (kJ/mol).
$\Delta_{sub} H$: Enthalpy of sublimation at a given temperature (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
IE: Ionization energy (eV).
***log*P$_{oct/wat}$**: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).