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
InchiKey:	LKUDPHPHKOZXCD-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	COc1cc(OC)cc(OC)c1
Mol. weight [g/mol]:	168.19
CAS:	621-23-8

Physical Properties

Property code	Value	Unit	Source
affp	926.70	kJ/mol	NIST Webbook
basg	898.20	kJ/mol	NIST Webbook
gf	-196.95	kJ/mol	Joback Method
hf	-412.16	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hsub	100.60 ± 1.90	kJ/mol	NIST Webbook
hvap	68.20 ± 2.00	kJ/mol	NIST Webbook
ie	7.96	eV	NIST Webbook
log10ws	-2.68		Aqueous Solubility Prediction Method
logp	1.712		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1405.00		NIST Webbook
rinpol	1418.30		NIST Webbook
rinpol	1418.30		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2172.00		NIST Webbook
tb	528.70	K	NIST Webbook
tc	714.26	K	Joback Method
tf	326.32	K	Aqueous Solubility Prediction Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.91	J/mol×K	509.22	Joback Method
cpg	298.31	J/mol×K	543.39	Joback Method
cpg	310.28	J/mol×K	577.57	Joback Method
cpg	321.81	J/mol×K	611.74	Joback Method
cpg	332.87	J/mol×K	645.92	Joback Method
cpg	343.44	J/mol×K	680.09	Joback Method
cpg	353.50	J/mol×K	714.26	Joback Method
dvisc	0.0008604	Pa×s	309.34	Joback Method
dvisc	0.0005446	Pa×s	342.65	Joback Method
dvisc	0.0003738	Pa×s	375.97	Joback Method
dvisc	0.0002728	Pa×s	409.28	Joback Method
dvisc	0.0002088	Pa×s	442.59	Joback Method
dvisc	0.0001658	Pa×s	475.91	Joback Method
dvisc	0.0001358	Pa×s	509.22	Joback Method
hsubt	116.00 ± 1.90	kJ/mol	375.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C621238&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Construction of solid liquid phase diagrams in ternary systems by titration calorimetry: https://www.doi.org/10.1016/j.tca.2006.02.017

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp: Proton affinity

basg: Gas basicity

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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