Benzene, (trimethoxymethyl)-

Other names:	Orthobenzoic acid, trimethyl ester
	Methyl orthobenzoate
	Trimethyl orthobenzoate
Inchi:	InChI=1S/C10H14O3/c1-11-10(12-2,13-3)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	IECKAVQTURBPON-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	COC(OC)(OC)c1ccccc1
Mol. weight [g/mol]:	182.22
CAS:	707-07-3

Physical Properties

Property code	Value	Unit	Source
chs	-5444.00 ± 1.20	kJ/mol	NIST Webbook
gf	-166.43	kJ/mol	Joback Method
hf	-433.30 ± 1.30	kJ/mol	NIST Webbook
hf	-429.40 ± 5.20	kJ/mol	NIST Webbook
hfl	-485.80 ± 3.10	kJ/mol	NIST Webbook
hfs	-491.90 ± 1.20	kJ/mol	NIST Webbook
hfus	11.85	kJ/mol	Joback Method
hsub	58.62 ± 0.38	kJ/mol	NIST Webbook
hsub	58.60	kJ/mol	NIST Webbook
hvap	56.40	kJ/mol	NIST Webbook
hvap	56.40 ± 4.20	kJ/mol	NIST Webbook
hvap	59.90 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.53		Crippen Method
logp	1.736		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	518.91	K	Joback Method
tc	731.53	K	Joback Method
tf	297.99	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.47	J/mol×K	731.53	Joback Method
cpg	401.25	J/mol×K	696.09	Joback Method
cpg	389.27	J/mol×K	660.65	Joback Method
cpg	376.51	J/mol×K	625.22	Joback Method
cpg	362.97	J/mol×K	589.78	Joback Method
cpg	348.63	J/mol×K	554.35	Joback Method
cpg	333.47	J/mol×K	518.91	Joback Method
dvisc	0.0019253	Pa×s	297.99	Joback Method
dvisc	0.0001289	Pa×s	518.91	Joback Method
dvisc	0.0001704	Pa×s	482.09	Joback Method
dvisc	0.0002357	Pa×s	445.27	Joback Method
dvisc	0.0003457	Pa×s	408.45	Joback Method
dvisc	0.0005470	Pa×s	371.63	Joback Method
dvisc	0.0009577	Pa×s	334.81	Joback Method
hvapt	58.60 ± 0.40	kJ/mol	313.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.70	K	0.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C707073&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume