1,2,3-Trimethoxybenzene

Other names:	Methylsyringol
	Pyrogallol trimethyl ether
	Tri-O-methylpyrogallol
	Benzene, 1,2,3-trimethoxy-
	1,2,3-Trimethoxybenzene (methylsyringol)
Inchi:	InChI=1S/C9H12O3/c1-10-7-5-4-6-8(11-2)9(7)12-3/h4-6H,1-3H3
InchiKey:	CRUILBNAQILVHZ-UHFFFAOYSA-N
Formula:	C9H12O3
SMILES:	COc1cccc(OC)c1OC
Mol. weight [g/mol]:	168.19
CAS:	634-36-6

Physical Properties

Property code	Value	Unit	Source
gf	-196.95	kJ/mol	Joback Method
hf	-412.16	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hsub	98.00 ± 0.30	kJ/mol	NIST Webbook
hvap	46.46	kJ/mol	Joback Method
ie	8.20 ± 0.15	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	1.712		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1309.00		NIST Webbook
rinpol	1315.10		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1309.00		NIST Webbook
ripol	1987.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1971.00		NIST Webbook
tb	514.15 ± 1.00	K	NIST Webbook
tb	514.20	K	NIST Webbook
tc	714.26	K	Joback Method
tf	309.34	K	Joback 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	113.40 ± 0.30	kJ/mol	375.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C634366&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

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

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