3,4,5-TRIMETHOXYTOLUENE

Other names:	Toluene, 3,4,5-trimethoxy-
	1,2,3-Trimethoxy-5-methylbenzene
	3,4,5-Trimethoxytoluene
	5-Methyl-1,2,3-trimethoxybenzene
	Benzene, 5-methyl-1,2,3-trimethoxy
Inchi:	InChI=1S/C10H14O3/c1-7-5-8(11-2)10(13-4)9(6-7)12-3/h5-6H,1-4H3
InchiKey:	KCIZTNZGSBSSRM-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	COc1cc(C)cc(OC)c1OC
Mol. weight [g/mol]:	182.22

Physical Properties

Property code	Value	Unit	Source
hf	-381.43	kJ/mol	Cheméo Relay (1.0)
hfus	18.09	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Cheméo Relay (1.0)
ie	7.84	eV	Cheméo Relay (1.0)
log10ws	-2.28		Cheméo Relay (1.0)
logp	2.021		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1419.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
tb	523.02	K	Cheméo Relay (1.0)
tc	720.62	K	Cheméo Relay (1.0)
tf	330.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.15	J/mol×K	537.08	Joback Method
cpg	343.37	J/mol×K	570.94	Joback Method
cpg	356.13	J/mol×K	604.80	Joback Method
cpg	368.41	J/mol×K	638.66	Joback Method
cpg	380.18	J/mol×K	672.52	Joback Method
cpg	391.43	J/mol×K	706.39	Joback Method
cpg	402.12	J/mol×K	740.25	Joback Method
dvisc	0.0006822	Pa×s	333.13	Joback Method
dvisc	0.0004499	Pa×s	367.12	Joback Method
dvisc	0.0003184	Pa×s	401.11	Joback Method
dvisc	0.0002378	Pa×s	435.10	Joback Method
dvisc	0.0001853	Pa×s	469.10	Joback Method
dvisc	0.0001493	Pa×s	503.09	Joback Method
dvisc	0.0001237	Pa×s	537.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.70	K	0.70	NIST Webbook

Sources

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6443692&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
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