2,4,6-Trimethoxytoluene

Other names: Benzene, 1,3,5-trimethoxy-2-methyl-
Toluene, 2,4,6-trimethoxy-
1,3,5-Trimethoxy-2-methylbenzene
Inchi: InChI=1S/C10H14O3/c1-7-9(12-3)5-8(11-2)6-10(7)13-4/h5-6H,1-4H3
InchiKey: TZPKFPYZCMHDHL-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: COc1cc(OC)c(C)c(OC)c1
Mol. weight [g/mol]: 182.22
CAS: 14107-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-198.16	kJ/mol	Joback Method
hf	-444.27	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	49.35	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.021		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.90		NIST Webbook
tb	537.08	K	Joback Method
tc	740.25	K	Joback Method
tf	333.13	K	Joback Method
vc	0.541	m3/kmol	Joback Method

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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14107972&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume