3,4-Dimethoxytoluene

Other names:	Benzene, 1,2-dimethoxy-4-methyl- Homoveratrole Toluene, 3,4-dimethoxy- 1,2-Dimethoxy-4-methylbenzene 4-Methyl-1,2-dimethoxybenzene 4-Methylveratrol 4-Methylveratrole NSC 7378 Veratrole, 4-methyl- 1,2-Dimethoxy-4-methyl-benzene (4-methylveratrol) Methyl veratrol
Inchi:	InChI=1S/C9H12O2/c1-7-4-5-8(10-2)9(6-7)11-3/h4-6H,1-3H3
InchiKey:	GYPMBQZAVBFUIZ-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	COc1ccc(C)cc1OC
Mol. weight [g/mol]:	152.19
CAS:	494-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-91.95	kJ/mol	Joback Method
hf	-279.94	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
ie	7.95	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.012		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1246.00		NIST Webbook

rinpol	1195.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1204.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1807.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1798.00		NIST Webbook
tb	493.20	K	NIST Webbook
tb	493.15 ± 1.00	K	NIST Webbook
tb	493.15 ± 1.00	K	NIST Webbook
tc	693.63	K	Joback Method
tf	287.11	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.85	J/mol×K	486.80	Joback Method
cpg	275.38	J/mol×K	521.27	Joback Method
cpg	287.43	J/mol×K	555.74	Joback Method
cpg	299.00	J/mol×K	590.21	Joback Method
cpg	310.08	J/mol×K	624.69	Joback Method
cpg	320.65	J/mol×K	659.16	Joback Method
cpg	330.70	J/mol×K	693.63	Joback Method
dvisc	0.0010774	Pa×s	287.11	Joback Method
dvisc	0.0006652	Pa×s	320.39	Joback Method
dvisc	0.0004497	Pa×s	353.67	Joback Method
dvisc	0.0003252	Pa×s	386.95	Joback Method
dvisc	0.0002475	Pa×s	420.24	Joback Method
dvisc	0.0001961	Pa×s	453.52	Joback Method
dvisc	0.0001604	Pa×s	486.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494995&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

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
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