1,2,4-Trimethoxybenzene

Other names: Benzene, 1,2,4-trimethoxy-
Inchi: InChI=1S/C9H12O3/c1-10-7-4-5-8(11-2)9(6-7)12-3/h4-6H,1-3H3
InchiKey: AGIQIOSHSMJYJP-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: COc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 168.19
CAS: 135-77-3

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
hvap	46.46	kJ/mol	Joback Method
ie	7.50 ± 0.15	eV	NIST Webbook
ie	7.49	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	1331.30		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1377.80		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2133.00		NIST Webbook
ripol	2094.00		NIST Webbook
tb	520.20	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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C135773&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