1,2,3,4-Tetramethoxybenzene

Inchi: InChI=1S/C10H14O4/c1-11-7-5-6-8(12-2)10(14-4)9(7)13-3/h5-6H,1-4H3
InchiKey: QCNHIJXDZKTWSA-UHFFFAOYSA-N
Formula: C10H14O4
SMILES: COc1ccc(OC)c(OC)c1OC
Mol. weight [g/mol]: 198.22
CAS: 21450-56-6

Physical Properties

Property code	Value	Unit	Source
gf	-303.16	kJ/mol	Joback Method
hf	-576.49	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.721		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2279.00		NIST Webbook
ripol	2321.00		NIST Webbook
tb	559.50	K	Joback Method
tc	760.80	K	Joback Method
tf	355.36	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.24	J/mol×K	559.50	Joback Method
cpg	367.38	J/mol×K	593.05	Joback Method
cpg	380.09	J/mol×K	626.60	Joback Method
cpg	392.32	J/mol×K	660.15	Joback Method

cpg	404.06	J/mol×K	693.70	Joback Method
cpg	415.25	J/mol×K	727.25	Joback Method
cpg	425.87	J/mol×K	760.80	Joback Method
dvisc	0.0005369	Pa×s	355.36	Joback Method
dvisc	0.0003605	Pa×s	389.38	Joback Method
dvisc	0.0002580	Pa×s	423.41	Joback Method
dvisc	0.0001941	Pa×s	457.43	Joback Method
dvisc	0.0001519	Pa×s	491.45	Joback Method
dvisc	0.0001227	Pa×s	525.48	Joback Method
dvisc	0.0001017	Pa×s	559.50	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21450566&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

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

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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