3,4-(Methylenedioxy)toluene

Other names: 1,3-Benzodioxole, 5-methyl-
5-methyl-1,3-benzodioxole
Inchi: InChI=1S/C8H8O2/c1-6-2-3-7-8(4-6)10-5-9-7/h2-4H,5H2,1H3
InchiKey: GHPODDMCSOYWNE-UHFFFAOYSA-N
Formula: C8H8O2
SMILES: Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 136.15
CAS: 7145-99-5

Physical Properties

Property code	Value	Unit	Source
gf	5.85	kJ/mol	Joback Method
hf	-165.72	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	54.90 ± 1.20	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.724		Crippen Method
mcvol	100.700	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	472.70	K	NIST Webbook
tc	713.45	K	Joback Method
tf	306.70	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.69	J/mol×K	484.39	Joback Method
cpg	226.38	J/mol×K	522.57	Joback Method
cpg	237.23	J/mol×K	560.74	Joback Method
cpg	247.29	J/mol×K	598.92	Joback Method
cpg	256.62	J/mol×K	637.10	Joback Method
cpg	265.27	J/mol×K	675.27	Joback Method
cpg	273.30	J/mol×K	713.45	Joback Method

dvisc	0.0019633	Pa×s	306.70	Joback Method
dvisc	0.0013990	Pa×s	336.31	Joback Method
dvisc	0.0010531	Pa×s	365.93	Joback Method
dvisc	0.0008272	Pa×s	395.54	Joback Method
dvisc	0.0006720	Pa×s	425.16	Joback Method
dvisc	0.0005608	Pa×s	454.77	Joback Method
dvisc	0.0004785	Pa×s	484.39	Joback Method
hvapt	54.90	kJ/mol	298.15	Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.00 ± 1.00	K	1.90	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7145995&Units=SI

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

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

Experimental and Computational Thermochemistry of 1,3-Benzodioxole Derivatives: https://www.doi.org/10.1021/je700035m

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

hvapt: Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume