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

Physical Properties

Property code	Value	Unit	Source
hfus	22.76	kJ/mol	Joback Method
hvap	54.90 ± 1.20	kJ/mol	NIST Webbook
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-2.71		Cheméo Relay (1.0)
logp	1.724		Crippen Method
mcvol	100.700	ml/mol	McGowan Method
tb	472.70	K	NIST Webbook
tf	283.54	K	Cheméo Relay (1.0)

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	336.32	Joback Method
dvisc	0.0010531	Pa×s	365.93	Joback Method
dvisc	0.0008272	Pa×s	395.55	Joback Method
dvisc	0.0006720	Pa×s	425.16	Joback Method

dvisc	0.0005608	Pa×s	454.78	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

Cheméo Relay (1.0, beta):

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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point