1,3-Benzodioxole

Other names:	Benzene, 1,2-(methylenedioxy)-
	(Methylenedioxy)benzene
	o-Methylenedioxybenzene
	Benzene, 1,2-[methylenebis(oxy)]-
	Benzodioxole
	1,2-(Methylenedioxy)benzene
	1,3-Dioxaindan
	1,3-Dioxindan
	3,4-Methylenedioxybenzene
	2H-1,3-Benzodioxole
	NSC 30095
	1,3-benzodioxolane
Inchi:	InChI=1S/C7H6O2/c1-2-4-7-6(3-1)8-5-9-7/h1-4H,5H2
InchiKey:	FTNJQNQLEGKTGD-UHFFFAOYSA-N
Formula:	C7H6O2
SMILES:	c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	122.12
CAS:	274-09-9

Physical Properties

Property code	Value	Unit	Source
chl	-3428.00 ± 2.00	kJ/mol	NIST Webbook
gf	7.06	kJ/mol	Joback Method
hf	-133.61	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	41.40	kJ/mol	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.21	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.415		Crippen Method
mcvol	86.610	ml/mol	McGowan Method
pc	4897.06	kPa	Joback Method
ripol	1530.00		NIST Webbook
ripol	1531.00		NIST Webbook
tb	445.70	K	NIST Webbook
tc	688.03	K	Joback Method
tf	282.91	K	Joback Method

vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.58	J/mol×K	456.53	Joback Method
cpg	185.56	J/mol×K	495.11	Joback Method
cpg	195.66	J/mol×K	533.70	Joback Method
cpg	204.93	J/mol×K	572.28	Joback Method
cpg	213.44	J/mol×K	610.86	Joback Method
cpg	221.26	J/mol×K	649.45	Joback Method
cpg	228.44	J/mol×K	688.03	Joback Method
dvisc	0.0023229	Pa×s	282.91	Joback Method
dvisc	0.0015997	Pa×s	311.85	Joback Method
dvisc	0.0011737	Pa×s	340.78	Joback Method
dvisc	0.0009039	Pa×s	369.72	Joback Method
dvisc	0.0007230	Pa×s	398.66	Joback Method
dvisc	0.0005961	Pa×s	427.59	Joback Method
dvisc	0.0005036	Pa×s	456.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.00 ± 1.00	K	2.70	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C274099&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume