

1,4-Benzodioxin, 2,3-dihydro-

Other names:	1,4-Benzodioxan Benzene, 1,2-[1,2-ethanediylbis(oxy)]- Ethylene o-phenylene dioxide Pyrocatechol ethylene ether 1,2-(Ethylenedioxy)benzene 1,4-Benzodioxane 1,4-Dioxatetralin
Inchi:	InChI=1S/C8H8O2/c1-2-4-8-7(3-1)9-5-6-10-8/h1-4H,5-6H2
InchiKey:	BNBQRQQYDMDJAH-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	c1ccc2c(c1)OCCO2
Mol. weight [g/mol]:	136.15
CAS:	493-09-4

Physical Properties

Property code	Value	Unit	Source
chl	-4036.70 ± 1.30	kJ/mol	NIST Webbook
gf	3.38	kJ/mol	Joback Method
hf	-160.41	kJ/mol	Joback Method
hfus	21.05	kJ/mol	Joback Method
hvap	67.40 ± 1.70	kJ/mol	NIST Webbook
hvap	50.42	kJ/mol	NIST Webbook
log10ws	-1.61		Crippen Method
logp	1.458		Crippen Method
mcvol	100.700	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
ripol	1800.00		NIST Webbook
tb	483.68	K	Joback Method
tc	720.55	K	Joback Method
tf	290.66	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.77	J/mol×K	483.68	Joback Method
cpg	226.87	J/mol×K	523.16	Joback Method
cpg	238.97	J/mol×K	562.64	Joback Method
cpg	250.14	J/mol×K	602.12	Joback Method
cpg	260.44	J/mol×K	641.59	Joback Method
cpg	269.93	J/mol×K	681.07	Joback Method
cpg	278.67	J/mol×K	720.55	Joback Method
dvisc	0.0030174	Pa×s	290.66	Joback Method
dvisc	0.0018387	Pa×s	322.83	Joback Method
dvisc	0.0012257	Pa×s	355.00	Joback Method
dvisc	0.0008740	Pa×s	387.17	Joback Method
dvisc	0.0006564	Pa×s	419.34	Joback Method
dvisc	0.0005135	Pa×s	451.51	Joback Method
dvisc	0.0004151	Pa×s	483.68	Joback Method
hvapt	50.40	kJ/mol	443.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	0.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493094&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

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
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
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

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