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

Other names:	1,4-Benzodioxan-2-hydroxymethyl
	1,4-Benzodioxan-2-methanol
	1,4-benzodioxane-2-methanol
	2-Hydroxymethyl-1,4-benzodioxan
	2-hydroxymethyl-1,4-benzodioxane
Inchi:	InChI=1S/C9H10O3/c10-5-7-6-11-8-3-1-2-4-9(8)12-7/h1-4,7,10H,5-6H2
InchiKey:	GWQOQQVKVOOHTI-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	OCC1COc2ccccc2O1
Mol. weight [g/mol]:	166.17
CAS:	3663-82-9

Physical Properties

Property code	Value	Unit	Source
gf	-132.73	kJ/mol	Joback Method
hf	-353.62	kJ/mol	Joback Method
hfus	28.78	kJ/mol	Experimental and computational thermochemistry of 1,4-benzodioxan and its 2-R derivatives
hsub	106.90 ± 0.80	kJ/mol	NIST Webbook
hvap	64.35	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.819		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	594.07	K	Joback Method
tc	808.44	K	Joback Method
tf	358.51	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	366.28	J/mol×K	808.44	Joback Method
cpg	358.14	J/mol×K	772.71	Joback Method
cpg	349.39	J/mol×K	736.98	Joback Method
cpg	339.98	J/mol×K	701.25	Joback Method
cpg	329.88	J/mol×K	665.53	Joback Method
cpg	319.04	J/mol×K	629.80	Joback Method
cpg	307.41	J/mol×K	594.07	Joback Method
dvisc	0.0045913	Pa×s	358.51	Joback Method
dvisc	0.0001643	Pa×s	594.07	Joback Method
dvisc	0.0002352	Pa×s	554.81	Joback Method
dvisc	0.0003556	Pa×s	515.55	Joback Method
dvisc	0.0005754	Pa×s	476.29	Joback Method
dvisc	0.0010154	Pa×s	437.03	Joback Method
dvisc	0.0020042	Pa×s	397.77	Joback Method
hfust	28.78	kJ/mol	362.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3663829&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 1,4-benzodioxan and its 2-R derivatives:	https://www.doi.org/10.1016/j.jct.2008.06.003
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume