1,3-BENZODIOXOLE-5-METHANOL

Other names:	1,3-Benzodioxole-5-methanol
	Benzyl alcohol, 3,4-(methylenedioxy)-
	Piperonol
	1-Hydroxymethyl-3,4-methylenedioxybenzene
	3,4-Methylenedioxybenzyl alcohol
	5-Hydroxymethyl-1,3-benzodioxole
	3,4-(Methylenedioxy)benzenemethanol
	1,3-Benzodioxol-5-ylmethanol
	NSC 26265
Inchi:	InChI=1S/C8H8O3/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-3,9H,4-5H2
InchiKey:	BHUIUXNAPJIDOG-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	OCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	152.15

Physical Properties

Property code	Value	Unit	Source
hfus	26.85	kJ/mol	Joback Method
hsub	103.70 ± 0.70	kJ/mol	NIST Webbook
hvap	80.70	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
logp	0.908		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
tb	528.16	K	Cheméo Relay (1.0)
tf	321.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.48	J/mol×K	788.41	Joback Method
cpg	291.82	J/mol×K	717.80	Joback Method
cpg	258.15	J/mol×K	576.57	Joback Method
cpg	267.48	J/mol×K	611.88	Joback Method

cpg	276.17	J/mol×K	647.18	Joback Method
cpg	284.27	J/mol×K	682.49	Joback Method
cpg	298.88	J/mol×K	753.10	Joback Method
dvisc	0.0036357	Pa×s	367.52	Joback Method
dvisc	0.0018360	Pa×s	402.36	Joback Method
dvisc	0.0010338	Pa×s	437.20	Joback Method
dvisc	0.0006336	Pa×s	472.05	Joback Method
dvisc	0.0004154	Pa×s	506.89	Joback Method
dvisc	0.0002875	Pa×s	541.73	Joback Method
dvisc	0.0002080	Pa×s	576.57	Joback Method
hfust	18.05	kJ/mol	327.10	NIST Webbook
hsubt	103.00 ± 0.60	kJ/mol	312.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.00 ± 1.00	K	2.70	NIST Webbook

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C495761&Units=SI

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hfus: Enthalpy of fusion at standard conditions

hfust: Enthalpy of fusion at a given temperature

hsub: Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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