

Piperonyl alcohol

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
CAS:	495-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-130.97	kJ/mol	Joback Method
hf	-317.95	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hsub	103.70 ± 0.70	kJ/mol	NIST Webbook
hvap	62.92	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	0.908		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	576.57	K	Joback Method
tc	788.41	K	Joback Method
tf	367.52	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	291.82	J/mol×K	717.80	Joback Method
cpg	298.88	J/mol×K	753.10	Joback Method
cpg	305.48	J/mol×K	788.41	Joback Method
dvisc	0.0018360	Pa×s	402.36	Joback Method
dvisc	0.0036357	Pa×s	367.52	Joback Method
dvisc	0.0010338	Pa×s	437.20	Joback Method
dvisc	0.0006336	Pa×s	472.04	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

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=C495761&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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