Piperonal

Other names:	1,3-Benzodioxole-5-carboxaldehyde
	3,4-(Methylenedioxy)benzaldehyde
	3,4-Bis(methylenedioxy)benzaldehyde
	3,4-Dihydroxybenzaldehyde methylene ketal
	3,4-Dimethylenedioxybenzaldehyde
	3,4-Methylene-dihydroxybenzaldehyde
	5-Formyl-1,3-benzodioxole
	Benzaldehyde, 3,4-(methylenedioxy)-
	Dioxymethylene-protocatechuic aldehyde
	Geliotropin
	Heliotropin
	Heliotropine
	Heliotropine (Piperonal)
	NSC 26826
	Piperanal
	Piperonaldehyde
	Piperonylaldehyde
	Protocatechuic aldehyde methylene ether
Inchi:	InChI=1S/C8H6O3/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-4H,5H2
InchiKey:	SATCULPHIDQDRE-UHFFFAOYSA-N
Formula:	C8H6O3
SMILES:	O=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	150.13
CAS:	120-57-0

Physical Properties

Property code	Value	Unit	Source
chs	-3645.00	kJ/mol	NIST Webbook
gf	-93.67	kJ/mol	Joback Method
hf	-251.30	kJ/mol	Joback Method
hfs	-363.00	kJ/mol	NIST Webbook
hfus	25.05	kJ/mol	Joback Method
hvap	52.96	kJ/mol	Joback Method
log10ws	-1.63		Estimated Solubility Method
log10ws	-1.63		Aqueous Solubility Prediction Method

logp	1.228		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	1329.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1285.40		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1292.20		NIST Webbook
rinpol	1285.10		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1347.00		NIST Webbook
ripol	2213.70		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2244.00		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2225.00		NIST Webbook
tb	536.00 ± 1.00	K	NIST Webbook
tb	536.20	K	NIST Webbook
tc	765.82	K	Joback Method
tf	310.25 ± 1.00	K	NIST Webbook
tf	309.65	K	Aqueous Solubility Prediction Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.91	J/mol×K	533.05	Joback Method

cpg	238.94	J/mol×K	571.85	Joback Method
cpg	248.18	J/mol×K	610.64	Joback Method
cpg	256.69	J/mol×K	649.44	Joback Method
cpg	264.53	J/mol×K	688.23	Joback Method
cpg	271.76	J/mol×K	727.03	Joback Method
cpg	278.44	J/mol×K	765.82	Joback Method
dvisc	0.0017306	Pa×s	379.42	Joback Method
dvisc	0.0023805	Pa×s	348.70	Joback Method
dvisc	0.0013198	Pa×s	410.15	Joback Method
dvisc	0.0010452	Pa×s	440.88	Joback Method
dvisc	0.0008533	Pa×s	471.60	Joback Method
dvisc	0.0007141	Pa×s	502.32	Joback Method
dvisc	0.0006100	Pa×s	533.05	Joback Method
hsubt	90.80	kJ/mol	323.00	NIST Webbook
hvapt	60.60	kJ/mol	448.00	NIST Webbook
hvapt	65.70	kJ/mol	331.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.00	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C120570&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chs: Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
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