1,3-Benzodioxole, 5-propyl-

Other names:	Benzene, 1,2-(methylenedioxy)-4-propyl-
	[1,2-(Methylenedioxy)-4-propyl]benzene
	Dihydrosafrol
	Dihydrosafrole
	2',3'-Dihydrosafrole
	5-Propyl-1,3-benzodioxole
	1-(3,4-Methylenedioxyphenyl)propane
	Safrole, dihydro-
	4-Propyl-1,2-(methylenedioxy)benzene
	Rcra waste number U090
	NSC 27867
Inchi:	InChI=1S/C10H12O2/c1-2-3-8-4-5-9-10(6-8)12-7-11-9/h4-6H,2-3,7H2,1H3
InchiKey:	MYEIDJPOUKASEC-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	164.20
CAS:	94-58-6

Physical Properties

Property code	Value	Unit	Source
gf	22.69	kJ/mol	Joback Method
hf	-207.00	kJ/mol	Joback Method
hfus	27.94	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.368		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1822.00		NIST Webbook
tb	530.15	K	Joback Method
tc	751.36	K	Joback Method
tf	329.24	K	Joback Method

vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.48	J/mol×K	530.15	Joback Method
cpg	314.21	J/mol×K	567.02	Joback Method
cpg	327.03	J/mol×K	603.89	Joback Method
cpg	338.99	J/mol×K	640.76	Joback Method
cpg	350.16	J/mol×K	677.63	Joback Method
cpg	360.59	J/mol×K	714.49	Joback Method
cpg	370.34	J/mol×K	751.36	Joback Method
dvisc	0.0021652	Pa×s	329.24	Joback Method
dvisc	0.0014752	Pa×s	362.73	Joback Method
dvisc	0.0010724	Pa×s	396.21	Joback Method
dvisc	0.0008193	Pa×s	429.69	Joback Method
dvisc	0.0006508	Pa×s	463.18	Joback Method
dvisc	0.0005333	Pa×s	496.66	Joback Method
dvisc	0.0004481	Pa×s	530.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.50 ± 0.50	K	2.40	NIST Webbook

Sources

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=C94586&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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
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