Safrole

Other names:	(1,2-(Methylenedioxy)-4-allyl)benzene 1,3-Benzodioxole, 5-(2-propen-1-yl)- 1,3-Benzodioxole, 5-(2-propenyl)- 1,3-Benzodioxole, 5-allyl- 1-Allyl-3,4-(methylenedioxy)benzene 3,4-(Methylenedioxy)allylbenzene 3,4-methylenedioxy-allylbenzene 3-(3,4-Methylenedioxyphenyl)prop-1-ene 4-allyl-1,2-(methylenedioxy)benzene 4-allyl-1,2-methylenedioxybenzene 4-allylpyrocatechol formaldehyde acetal 5-(2-propenyl)-1,3-benzodioxole 5-Allyl-1,3-benzodioxole Allylcatechol methylene ether Allyldioxybenzene methylene ether Allylpyrocatechol methylene ether Benzene, 4-allyl-1,2-(methylenedioxy)- NSC 11831 Rcra waste number U203 Rhyuno oil Safrene Safrole MF Shikimole Shikomol benzene, 1,2-methylenedioxy-4-(2-propenyl)- benzene, 1,2-methylenedioxy-4-allyl- m-Allylpyrocatechin methylene ether safrol
Inchi:	InChI=1S/C10H10O2/c1-2-3-8-4-5-9-10(6-8)12-7-11-9/h2,4-6H,1,3,7H2
InchiKey:	ZMQAAUBTXCXRIC-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	C=CCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	162.19
CAS:	94-59-7

Physical Properties

Property code	Value	Unit	Source

gf	110.53	kJ/mol	Joback Method
hf	-81.57	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.144		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1293.20		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1291.40		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1286.00		NIST Webbook

rinpol	1286.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1296.00	NIST Webbook
rinpol	1260.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1289.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1280.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1264.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1286.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1285.00	NIST Webbook
rinpol	1259.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1289.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1284.00	NIST Webbook
rinpol	1264.50	NIST Webbook
rinpol	1269.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1278.00	NIST Webbook
rinpol	218.98	NIST Webbook
rinpol	219.88	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1285.00	NIST Webbook

rinpol	1265.00		NIST Webbook
rinpol	218.98		NIST Webbook
rinpol	1264.50		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1290.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1874.00		NIST Webbook
ripol	1874.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1873.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1869.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1874.00		NIST Webbook
tb	509.05 ± 1.00	K	NIST Webbook
tb	504.80 ± 0.20	K	NIST Webbook
tb	509.10 ± 0.50	K	NIST Webbook
tb	509.05 ± 0.40	K	NIST Webbook
tb	506.20	K	NIST Webbook
tc	753.00	K	Joback Method
tf	327.48	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.85	J/mol×K	526.83	Joback Method
cpg	294.85	J/mol×K	564.53	Joback Method

cpg	306.92	J/mol×K	602.22	Joback Method
cpg	318.11	J/mol×K	639.92	Joback Method
cpg	328.50	J/mol×K	677.61	Joback Method
cpg	338.15	J/mol×K	715.31	Joback Method
cpg	347.13	J/mol×K	753.00	Joback Method
dvisc	0.0020555	Pa×s	327.48	Joback Method
dvisc	0.0014246	Pa×s	360.71	Joback Method
dvisc	0.0010504	Pa×s	393.93	Joback Method
dvisc	0.0008120	Pa×s	427.16	Joback Method
dvisc	0.0006515	Pa×s	460.38	Joback Method
dvisc	0.0005385	Pa×s	493.61	Joback Method
dvisc	0.0004559	Pa×s	526.83	Joback Method
hvapt	54.60	kJ/mol	421.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.70	K	0.80	NIST Webbook
tbrp	377.50 ± 0.50	K	0.80	NIST Webbook

Sources

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

Phase Equilibria of the Systems CO2 + Styrene, CO2 + Safrole, and CO2 + Styrene + Safrole: https://www.doi.org/10.1021/je400110c

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=C94597&Units=SI

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

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
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