4-Methoxysafrole

Other names:	5-methoxy-6-(2-propenyl)-1,3-benzodioxole
	Asaricin
	Sarisane
	Benzene, 1-allyl-2-methoxy-4,5-methylenedioxy
Inchi:	InChI=1S/C11H12O3/c1-3-4-8-5-10-11(14-7-13-10)6-9(8)12-2/h3,5-6H,1,4,7H2,2H3
InchiKey:	FYRHTIWFKXZWAD-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	C=CCc1cc2c(cc1OC)OCO2
Mol. weight [g/mol]:	192.21
CAS:	18607-93-7

Physical Properties

Property code	Value	Unit	Source
gf	4.32	kJ/mol	Joback Method
hf	-245.90	kJ/mol	Joback Method
hfus	30.05	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.152		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2187.00		NIST Webbook
ripol	2187.00		NIST Webbook
tb	577.11	K	Joback Method
tc	797.56	K	Joback Method
tf	373.50	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.04	J/mol×K	577.11	Joback Method
cpg	363.26	J/mol×K	613.85	Joback Method
cpg	375.67	J/mol×K	650.59	Joback Method
cpg	387.31	J/mol×K	687.33	Joback Method
cpg	398.23	J/mol×K	724.07	Joback Method
cpg	408.46	J/mol×K	760.81	Joback Method
cpg	418.05	J/mol×K	797.56	Joback Method
dvisc	0.0014201	Pa×s	373.50	Joback Method
dvisc	0.0010235	Pa×s	407.44	Joback Method
dvisc	0.0007758	Pa×s	441.37	Joback Method
dvisc	0.0006118	Pa×s	475.31	Joback Method
dvisc	0.0004980	Pa×s	509.24	Joback Method
dvisc	0.0004159	Pa×s	543.17	Joback Method
dvisc	0.0003548	Pa×s	577.11	Joback Method

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=C18607937&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume