Benzene, 1,2-(methylenedioxy)-4-propenyl-, (E)-

Other names: 1,3-Benzodioxole, 5-(1-propenyl)-, (E)-
«beta»-Isosafrole
(E)-Isosafrole
trans-Isosafrole
trans-1,2-(Methylenedioxy)-4-propenylbenzene
(E)-Isosafrol

Inchi: InChI=1S/C10H10O2/c1-2-3-8-4-5-9-10(6-8)12-7-11-9/h2-6H,7H2,1H3/b3-2+

InchiKey: VHVOLFRBFDOUSH-NSCUHMNNSA-N

Formula: C10H10O2

SMILES: CC=Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 162.19

CAS: 4043-71-4

Physical Properties

Property code	Value	Unit	Source
gf	102.91	kJ/mol	Joback Method
hf	-89.78	kJ/mol	Joback Method
hfus	28.14	kJ/mol	Joback Method
hvap	50.65	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.448		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1374.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	534.31	K	Joback Method
tc	766.11	K	Joback Method
tf	324.16	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.89	J/mol×K	534.31	Joback Method

cpg	295.01	J/mol×K	572.94	Joback Method
cpg	307.14	J/mol×K	611.58	Joback Method
cpg	318.35	J/mol×K	650.21	Joback Method
cpg	328.73	J/mol×K	688.84	Joback Method
cpg	338.36	J/mol×K	727.47	Joback Method
cpg	347.33	J/mol×K	766.11	Joback Method
dvisc	0.0019464	Pa×s	324.16	Joback Method
dvisc	0.0012988	Pa×s	359.19	Joback Method
dvisc	0.0009313	Pa×s	394.21	Joback Method
dvisc	0.0007050	Pa×s	429.24	Joback Method
dvisc	0.0005566	Pa×s	464.26	Joback Method
dvisc	0.0004543	Pa×s	499.28	Joback Method
dvisc	0.0003807	Pa×s	534.31	Joback Method

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=C4043714&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume