1,3-Benzodioxole, 4,5-dimethoxy-6-(2-propenyl)-

Other names: Benzene, 1-allyl-2,3-dimethoxy-4,5-(methylenedioxy)-
Dill apiol
Dill apiole
1-Allyl-2,3-dimethoxy-4,5-methylenedioxybenzene

Inchi: InChI=1S/C12H14O4/c1-4-5-8-6-9-11(16-7-15-9)12(14-3)10(8)13-2/h4,6H,1,5,7H2,2-3H3

InchiKey: LIKYNOPXHGPMIH-UHFFFAOYSA-N

Formula: C12H14O4

SMILES: C=CCc1cc2c(c(OC)c1OC)OCO2

Mol. weight [g/mol]: 222.24

CAS: 484-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-101.89	kJ/mol	Joback Method
hf	-410.23	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.161		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1613.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1615.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1622.00		NIST Webbook

rinpol	1625.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1622.00	NIST Webbook
rinpol	1662.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1586.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1625.00	NIST Webbook
rinpol	1611.00	NIST Webbook
rinpol	1603.00	NIST Webbook
rinpol	1634.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1625.00	NIST Webbook
rinpol	1633.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1602.00	NIST Webbook
rinpol	1624.00	NIST Webbook
rinpol	1582.00	NIST Webbook
rinpol	1628.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1625.00	NIST Webbook
rinpol	1622.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1624.00	NIST Webbook
rinpol	1628.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1631.00	NIST Webbook
rinpol	1612.00	NIST Webbook
rinpol	1610.00	NIST Webbook
rinpol	1622.00	NIST Webbook
rinpol	1595.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1619.00	NIST Webbook
ripol	2310.00	NIST Webbook
ripol	2380.00	NIST Webbook
ripol	2305.00	NIST Webbook
ripol	2384.00	NIST Webbook
ripol	2384.00	NIST Webbook
ripol	2384.00	NIST Webbook
ripol	2380.00	NIST Webbook
ripol	2310.00	NIST Webbook

ripol	2338.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2370.00		NIST Webbook
tb	627.39	K	Joback Method
tc	842.34	K	Joback Method
tf	419.52	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.38	J/mol×K	627.39	Joback Method
cpg	434.89	J/mol×K	663.21	Joback Method
cpg	447.67	J/mol×K	699.04	Joback Method
cpg	459.71	J/mol×K	734.86	Joback Method
cpg	471.05	J/mol×K	770.69	Joback Method
cpg	481.71	J/mol×K	806.51	Joback Method
cpg	491.71	J/mol×K	842.34	Joback Method
dvisc	0.0009674	Pa×s	419.52	Joback Method
dvisc	0.0007188	Pa×s	454.17	Joback Method
dvisc	0.0005571	Pa×s	488.81	Joback Method
dvisc	0.0004466	Pa×s	523.46	Joback Method
dvisc	0.0003679	Pa×s	558.10	Joback Method
dvisc	0.0003101	Pa×s	592.75	Joback Method
dvisc	0.0002663	Pa×s	627.39	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=C484311&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