

Benzene, (1,2-dimethoxyethenyl)-, (Z)-

Inchi:	InChI=1S/C10H12O2/c1-11-8-10(12-2)9-6-4-3-5-7-9/h3-8H,1-2H3/b10-8-
InchiKey:	LKCWZGRTGFCUEH-NTMALXAHSA-N
Formula:	C10H12O2
SMILES:	COC=C(OC)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	50735-84-7

Physical Properties

Property code	Value	Unit	Source
gf	7.40	kJ/mol	Joback Method
hf	-170.21	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	44.99	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.278		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	503.76	K	Joback Method
tc	718.98	K	Joback Method
tf	254.30	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.01	J/mol×K	503.76	Joback Method
cpg	302.15	J/mol×K	539.63	Joback Method
cpg	315.54	J/mol×K	575.50	Joback Method
cpg	328.18	J/mol×K	611.37	Joback Method
cpg	340.09	J/mol×K	647.24	Joback Method
cpg	351.30	J/mol×K	683.11	Joback Method
cpg	361.82	J/mol×K	718.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50735847&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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