Benzene, (3,3-diethoxy-1-propynyl)-

Other names:	Propiolaldehyde, phenyl-, diethyl acetal
	Phenylpropargyl aldehyde diethyl acetal
	3-Phenylpropynal diethyl acetal
	3-Phenyl-2-propynyl aldehyde diethyl acetal
	Phenylpropiolic aldehyde diethylacetal
	dehydrocinnamaldehyde-diethylacetal
Inchi:	InChI=1S/C13H16O2/c1-3-14-13(15-4-2)11-10-12-8-6-5-7-9-12/h5-9,13H,3-4H2,1-2H3
InchiKey:	DTEGZYXCDQFSBZ-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	CCOC(C#Cc1ccccc1)OCC
Mol. weight [g/mol]:	204.26
CAS:	6142-95-6

Physical Properties

Property code	Value	Unit	Source
gf	161.35	kJ/mol	Joback Method
hf	-72.54	kJ/mol	Joback Method
hfus	25.44	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.437		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
tb	576.92	K	Joback Method
tc	798.58	K	Joback Method
tf	398.25	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.21	J/mol×K	576.92	Joback Method
cpg	426.81	J/mol×K	613.86	Joback Method
cpg	442.50	J/mol×K	650.81	Joback Method

cpg	457.28	J/mol×K	687.75	Joback Method
cpg	471.18	J/mol×K	724.69	Joback Method
cpg	484.20	J/mol×K	761.63	Joback Method
cpg	496.36	J/mol×K	798.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.70	K	0.30	NIST Webbook
tbrp	416.00	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6142956&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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume