BENZENE, (2,2-DIETHOXYETHYL)-

Other names:	Acetaldehyde, phenyl-, diethyl acetal
	Benzeneacetaldehyde, diethyl acetal
	Phenylacetaldehyde diethyl acetal
	1,1-diethoxy-2-phenylethane
	(2,2-diethoxyethyl)benzene
Inchi:	InChI=1S/C12H18O2/c1-3-13-12(14-4-2)10-11-8-6-5-7-9-11/h5-9,12H,3-4,10H2,1-2H3
InchiKey:	FYERTDTXGGOMGT-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCOC(Cc1ccccc1)OCC
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
af	0.4824		Cheméo Relay (1.0)
gf	-49.87	kJ/mol	Joback Method
hf	-330.62	kJ/mol	Cheméo Relay (1.0)
hfus	19.73	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-2.04		Cheméo Relay (1.0)
logp	2.628		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1711.00		NIST Webbook
tb	510.98	K	Cheméo Relay (1.0)
tc	698.43	K	Cheméo Relay (1.0)
tf	211.37	K	Cheméo Relay (1.0)
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.63	J/mol×K	545.04	Joback Method
cpg	415.09	J/mol×K	578.41	Joback Method
cpg	430.74	J/mol×K	611.77	Joback Method
cpg	445.59	J/mol×K	645.14	Joback Method
cpg	459.67	J/mol×K	678.50	Joback Method
cpg	472.98	J/mol×K	711.87	Joback Method
cpg	485.53	J/mol×K	745.23	Joback Method
dvisc	0.0027402	Pa×s	280.88	Joback Method
dvisc	0.0011747	Pa×s	324.91	Joback Method
dvisc	0.0006164	Pa×s	368.93	Joback Method
dvisc	0.0003711	Pa×s	412.96	Joback Method
dvisc	0.0002464	Pa×s	456.99	Joback Method
dvisc	0.0001758	Pa×s	501.01	Joback Method
dvisc	0.0001324	Pa×s	545.04	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6314972&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
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