Benzaldehyde diethylacetal

Other names:	Benzene, (diethoxymethyl)- Toluene, «alpha»,«alpha»-diethoxy- (Diethoxymethyl)benzene «alpha»,«alpha»-diethoxytoluene
Inchi:	InChI=1S/C11H16O2/c1-3-12-11(13-4-2)10-8-6-5-7-9-10/h5-9,11H,3-4H2,1-2H3
InchiKey:	MAQMEXSLUSZDQM-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCOC(OCC)c1ccccc1
Mol. weight [g/mol]:	180.24
CAS:	774-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-58.29	kJ/mol	Joback Method
hf	-303.56	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	62.80 ± 0.60	kJ/mol	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.758		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1291.00		NIST Webbook
tb	494.00 ± 5.00	K	NIST Webbook
tb	492.00 ± 2.00	K	NIST Webbook
tc	725.26	K	Joback Method
tf	269.61	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.33	J/mol×K	522.16	Joback Method
cpg	366.99	J/mol×K	556.01	Joback Method
cpg	381.91	J/mol×K	589.86	Joback Method
cpg	396.07	J/mol×K	623.71	Joback Method
cpg	409.51	J/mol×K	657.56	Joback Method
cpg	422.21	J/mol×K	691.41	Joback Method
cpg	434.19	J/mol×K	725.26	Joback Method
dvisc	0.0028409	Pa×s	269.61	Joback Method
dvisc	0.0012360	Pa×s	311.70	Joback Method
dvisc	0.0006555	Pa×s	353.79	Joback Method
dvisc	0.0003978	Pa×s	395.88	Joback Method
dvisc	0.0002658	Pa×s	437.98	Joback Method
dvisc	0.0001906	Pa×s	480.07	Joback Method
dvisc	0.0001442	Pa×s	522.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C774481&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
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