

1,3-Diethoxybenzene

Other names:	m-Diethoxybenzene Benzene, 1,3-diethoxy-
Inchi:	InChI=1S/C10H14O2/c1-3-11-9-6-5-7-10(8-9)12-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	MKGFYMKFBCWNCP-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCOc1cccc(OCC)c1
Mol. weight [g/mol]:	166.22
CAS:	2049-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-73.90	kJ/mol	Joback Method
hf	-289.11	kJ/mol	Joback Method
hfus	17.68	kJ/mol	Joback Method
hvap	45.61	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.484		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	508.00	K	NIST Webbook
tc	707.41	K	Joback Method
tf	285.50	K	NIST Webbook
vc	0.523	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.97	J/molxK	504.70	Joback Method
cpg	319.97	J/molxK	538.49	Joback Method
cpg	333.36	J/molxK	572.27	Joback Method
cpg	346.16	J/molxK	606.06	Joback Method
cpg	358.34	J/molxK	639.84	Joback Method
cpg	369.93	J/molxK	673.63	Joback Method
cpg	380.91	J/molxK	707.41	Joback Method

dvisc	0.0014900	Paxs	285.86	Joback Method
dvisc	0.0008299	Paxs	322.33	Joback Method
dvisc	0.0005207	Paxs	358.81	Joback Method
dvisc	0.0003560	Paxs	395.28	Joback Method
dvisc	0.0002596	Paxs	431.75	Joback Method
dvisc	0.0001988	Paxs	468.23	Joback Method
dvisc	0.0001582	Paxs	504.70	Joback Method

Sources

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=C2049732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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