

O-DIETHOXYBENZENE

Other names:	o-Diethoxy benzene Benzene, 1,2-diethoxy- Benzene, o-diethoxy- Catechol diethyl ether
Inchi:	InChI=1S/C10H14O2/c1-3-11-9-7-5-6-8-10(9)12-4-2/h5-8H,3-4H2,1-2H3
InchiKey:	QZYDOKBVZJLQCK-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCOc1ccccc1OCC
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
af	0.5245		Cheméo Relay (1.0)
hf	-297.29	kJ/mol	Cheméo Relay (1.0)
hfus	17.68	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Cheméo Relay (1.0)
ie	8.09	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
logp	2.484		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1214.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	496.67	K	Cheméo Relay (1.0)
tc	691.81	K	Cheméo Relay (1.0)
tf	285.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.97	J/mol×K	504.70	Joback Method
cpg	319.97	J/mol×K	538.49	Joback Method
cpg	333.36	J/mol×K	572.27	Joback Method
cpg	346.16	J/mol×K	606.06	Joback Method

cpg	358.34	J/mol×K	639.84	Joback Method
cpg	369.93	J/mol×K	673.63	Joback Method
cpg	380.91	J/mol×K	707.41	Joback Method
dvisc	0.0014900	Pa×s	285.86	Joback Method
dvisc	0.0008299	Pa×s	322.33	Joback Method
dvisc	0.0005207	Pa×s	358.81	Joback Method
dvisc	0.0003560	Pa×s	395.28	Joback Method
dvisc	0.0002596	Pa×s	431.75	Joback Method
dvisc	0.0001988	Pa×s	468.23	Joback Method
dvisc	0.0001582	Pa×s	504.70	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050466&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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