

Benzene, 1,3-dimethoxy-2-ethyl

Inchi:	InChI=1S/C10H14O2/c1-4-8-9(11-2)6-5-7-10(8)12-3/h5-7H,4H2,1-3H3
InchiKey:	BXBOHCCJANHPMS-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCc1c(OC)cccc1OC
Mol. weight [g/mol]:	166.22

Physical Properties

Property code	Value	Unit	Source
gf	-83.53	kJ/mol	Joback Method
hf	-300.58	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.266		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1283.00		NIST Webbook
tb	509.68	K	Joback Method
tc	713.56	K	Joback Method
tf	298.38	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.17	J/mol×K	509.68	Joback Method
cpg	319.83	J/mol×K	543.66	Joback Method
cpg	332.95	J/mol×K	577.64	Joback Method
cpg	345.51	J/mol×K	611.62	Joback Method
cpg	357.50	J/mol×K	645.60	Joback Method
cpg	368.93	J/mol×K	679.58	Joback Method
cpg	379.79	J/mol×K	713.56	Joback Method
dvisc	0.0011096	Pa×s	298.38	Joback Method
dvisc	0.0006697	Pa×s	333.60	Joback Method

dvisc	0.0004451	Pa×s	368.81	Joback Method
dvisc	0.0003177	Pa×s	404.03	Joback Method
dvisc	0.0002393	Pa×s	439.25	Joback Method
dvisc	0.0001880	Pa×s	474.46	Joback Method
dvisc	0.0001528	Pa×s	509.68	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=R142813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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<https://www.chemeo.com/cid/39-325-8/Benzene-1-3-dimethoxy-2-ethyl.pdf>

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