

Benzene, 1,3-dimethoxy-4-ethyl

Inchi:	InChI=1S/C10H14O2/c1-4-8-5-6-9(11-2)7-10(8)12-3/h5-7H,4H2,1-3H3
InchiKey:	XRJYMHASJFSHRH-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCc1ccc(OC)cc1OC
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	1307.00		NIST Webbook
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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/molxK	509.68	Joback Method
cpg	319.83	J/molxK	543.66	Joback Method
cpg	332.95	J/molxK	577.64	Joback Method
cpg	345.51	J/molxK	611.62	Joback Method
cpg	357.50	J/molxK	645.60	Joback Method
cpg	368.93	J/molxK	679.58	Joback Method
cpg	379.79	J/molxK	713.56	Joback Method
dvisc	0.0011096	Paxs	298.38	Joback Method

dvisc	0.0006697	Paxs	333.60	Joback Method
dvisc	0.0004451	Paxs	368.81	Joback Method
dvisc	0.0003177	Paxs	404.03	Joback Method
dvisc	0.0002393	Paxs	439.25	Joback Method
dvisc	0.0001880	Paxs	474.46	Joback Method
dvisc	0.0001528	Paxs	509.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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