

Benzene, 1,3-dimethoxy-4-pentyl

Inchi:	InChI=1S/C13H20O2/c1-4-5-6-7-11-8-9-12(14-2)10-13(11)15-3/h8-10H,4-7H2,1-3H3
InchiKey:	APEKBFINQBGPJW-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CCCCCc1ccc(OC)cc1OC
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	-58.27	kJ/mol	Joback Method
hf	-362.50	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	52.95	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.436		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpola	1582.00		NIST Webbook
tb	578.32	K	Joback Method
tc	773.80	K	Joback Method
tf	332.19	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.62	J/molxK	578.32	Joback Method
cpg	521.59	J/molxK	741.22	Joback Method
cpg	508.24	J/molxK	708.64	Joback Method
cpg	494.16	J/molxK	676.06	Joback Method
cpg	479.37	J/molxK	643.48	Joback Method
cpg	463.86	J/molxK	610.90	Joback Method
cpg	534.23	J/molxK	773.80	Joback Method
dvisc	0.0001232	Paxs	578.32	Joback Method
dvisc	0.0001544	Paxs	537.30	Joback Method

dvisc	0.0002008	Paxs	496.28	Joback Method
dvisc	0.0002739	Paxs	455.25	Joback Method
dvisc	0.0003973	Paxs	414.23	Joback Method
dvisc	0.0006253	Paxs	373.21	Joback Method
dvisc	0.0011010	Paxs	332.19	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143103&Units=SI

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/55-127-0/Benzene-1-3-dimethoxy-4-pentyl.pdf>

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