

Benzene, 1,3-dimethoxy-4-octyl

Inchi:	InChI=1S/C16H26O2/c1-4-5-6-7-8-9-10-14-11-12-15(17-2)13-16(14)18-3/h11-13H,4-10H
InchiKey:	ZYLKETAKQZGRHA-UHFFFAOYSA-N
Formula:	C16H26O2
SMILES:	CCCCCCCCc1ccc(OC)cc1OC
Mol. weight [g/mol]:	250.38

Physical Properties

Property code	Value	Unit	Source
gf	-33.01	kJ/mol	Joback Method
hf	-424.42	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.607		Crippen Method
mvol	224.280	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
tb	646.96	K	Joback Method
tc	835.82	K	Joback Method
tf	366.00	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.00	J/molxK	646.96	Joback Method
cpg	684.93	J/molxK	804.35	Joback Method
cpg	670.42	J/molxK	772.87	Joback Method
cpg	655.07	J/molxK	741.39	Joback Method
cpg	638.89	J/molxK	709.91	Joback Method
cpg	621.87	J/molxK	678.44	Joback Method
cpg	698.63	J/molxK	835.82	Joback Method
dvisc	0.0000922	Paxs	646.96	Joback Method

dvisc	0.0001172	Paxs	600.13	Joback Method
dvisc	0.0001552	Paxs	553.31	Joback Method
dvisc	0.0002165	Paxs	506.48	Joback Method
dvisc	0.0003232	Paxs	459.65	Joback Method
dvisc	0.0005285	Paxs	412.83	Joback Method
dvisc	0.0009798	Paxs	366.00	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143094&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/82-375-5/Benzene-1-3-dimethoxy-4-octyl.pdf>

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