

Benzene, 1,3-dimethoxy-2-octyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H26O2/c1-4-5-6-7-8-9-11-14-15(17-2)12-10-13-16(14)18-3/h10,12-13H,4-9

NJKIZYQPPYEBRG-UHFFFAOYSA-N

C16H26O2

CCCCCCCCc1c(OC)cccc1OC

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
mcvol	224.280	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	646.96	K	Joback Method
tc	835.82	K	Joback Method
tf	366.00	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.00	J/mol×K	646.96	Joback Method
cpg	621.87	J/mol×K	678.44	Joback Method
cpg	638.89	J/mol×K	709.91	Joback Method
cpg	655.07	J/mol×K	741.39	Joback Method
cpg	670.42	J/mol×K	772.87	Joback Method
cpg	684.93	J/mol×K	804.35	Joback Method
cpg	698.63	J/mol×K	835.82	Joback Method
dvisc	0.0009798	Pa×s	366.00	Joback Method

dvisc	0.0005285	Pa×s	412.83	Joback Method
dvisc	0.0003232	Pa×s	459.65	Joback Method
dvisc	0.0002165	Pa×s	506.48	Joback Method
dvisc	0.0001552	Pa×s	553.31	Joback Method
dvisc	0.0001172	Pa×s	600.13	Joback Method
dvisc	0.0000922	Pa×s	646.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142922&Units=SI
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

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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