Benzene, 1,3-dimethoxy-5-hexyl

Inchi: InChI=1S/C14H22O2/c1-4-5-6-7-8-12-9-13(15-2)11-14(10-12)16-3/h9-11H,4-8H2,1-3H3
InchiKey: PYDWBVCSEYGZTH-UHFFFAOYSA-N
Formula: C14H22O2
SMILES: CCCCCCc1cc(OC)cc(OC)c1
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-49.85	kJ/mol	Joback Method
hf	-383.14	kJ/mol	Joback Method
hfus	27.65	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.827		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	601.20	K	Joback Method
tc	794.21	K	Joback Method
tf	343.46	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.23	J/mol×K	601.20	Joback Method
cpg	515.10	J/mol×K	633.37	Joback Method
cpg	531.19	J/mol×K	665.54	Joback Method
cpg	546.53	J/mol×K	697.71	Joback Method
cpg	561.10	J/mol×K	729.87	Joback Method
cpg	574.91	J/mol×K	762.04	Joback Method
cpg	587.97	J/mol×K	794.21	Joback Method
dvisc	0.0010700	Pa×s	343.46	Joback Method

dvisc	0.0005968	Pa×s	386.42	Joback Method
dvisc	0.0003741	Pa×s	429.37	Joback Method
dvisc	0.0002553	Pa×s	472.33	Joback Method
dvisc	0.0001857	Pa×s	515.29	Joback Method
dvisc	0.0001419	Pa×s	558.24	Joback Method
dvisc	0.0001126	Pa×s	601.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143178&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