Benzene, 1,3-dimethoxy-2-methyl-4-pentyl

Inchi: InChI=1S/C14H22O2/c1-5-6-7-8-12-9-10-13(15-3)11(2)14(12)16-4/h9-10H,5-8H2,1-4H3
InchiKey: BJKIXSUOHIMKOW-UHFFFAOYSA-N
Formula: C14H22O2
SMILES: CCCCCc1ccc(OC)c(C)c1OC
Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	-59.48	kJ/mol	Joback Method
hf	-394.61	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	55.84	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.745		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	606.18	K	Joback Method
tc	800.12	K	Joback Method
tf	355.98	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.22	J/mol×K	606.18	Joback Method
cpg	514.89	J/mol×K	638.50	Joback Method
cpg	530.82	J/mol×K	670.83	Joback Method
cpg	546.01	J/mol×K	703.15	Joback Method
cpg	560.47	J/mol×K	735.47	Joback Method
cpg	574.18	J/mol×K	767.80	Joback Method
cpg	587.16	J/mol×K	800.12	Joback Method
dvisc	0.0008461	Pa×s	355.98	Joback Method

dvisc	0.0005050	Pa×s	397.68	Joback Method
dvisc	0.0003324	Pa×s	439.38	Joback Method
dvisc	0.0002352	Pa×s	481.08	Joback Method
dvisc	0.0001759	Pa×s	522.78	Joback Method
dvisc	0.0001373	Pa×s	564.48	Joback Method
dvisc	0.0001109	Pa×s	606.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142893&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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