

Benzene, 1,3-dimethoxy-5-methyl-2-pentyl

Inchi:	InChI=1S/C14H22O2/c1-5-6-7-8-12-13(15-3)9-11(2)10-14(12)16-4/h9-10H,5-8H2,1-4H3
InchiKey:	TXFZJLUODSWBKE-UHFFFAOYSA-N
Formula:	C14H22O2
SMILES:	CCCCC1c(OC)cc(C)cc1OC
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
mvol	196.100	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1604.00		NIST Webbook
tb	606.18	K	Joback Method
tc	800.12	K	Joback Method
tf	355.98	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.22	J/molxK	606.18	Joback Method
cpg	514.89	J/molxK	638.50	Joback Method
cpg	530.82	J/molxK	670.83	Joback Method
cpg	546.01	J/molxK	703.15	Joback Method
cpg	560.47	J/molxK	735.47	Joback Method
cpg	574.18	J/molxK	767.80	Joback Method
cpg	587.16	J/molxK	800.12	Joback Method
dvisc	0.0008461	Paxs	355.98	Joback Method
dvisc	0.0005050	Paxs	397.68	Joback Method

dvisc	0.0003324	Paxs	439.38	Joback Method
dvisc	0.0002352	Paxs	481.08	Joback Method
dvisc	0.0001759	Paxs	522.78	Joback Method
dvisc	0.0001373	Paxs	564.48	Joback Method
dvisc	0.0001109	Paxs	606.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143207&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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