

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

Inchi:	InChI=1S/C12H18O2/c1-5-6-10-7-8-11(13-3)9(2)12(10)14-4/h7-8H,5-6H2,1-4H3
InchiKey:	NRIXNYIKCHUTPF-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCc1ccc(OC)c(C)c1OC
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-76.32	kJ/mol	Joback Method
hf	-353.33	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.965		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	560.42	K	Joback Method
tc	759.59	K	Joback Method
tf	333.44	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.69	J/molxK	560.42	Joback Method
cpg	413.94	J/molxK	593.62	Joback Method
cpg	428.55	J/molxK	626.81	Joback Method
cpg	442.54	J/molxK	660.01	Joback Method
cpg	455.88	J/molxK	693.20	Joback Method
cpg	468.57	J/molxK	726.40	Joback Method
cpg	480.61	J/molxK	759.59	Joback Method
dvisc	0.0008729	Paxs	333.44	Joback Method

dvisc	0.0005412	Paxs	371.27	Joback Method
dvisc	0.0003666	Paxs	409.10	Joback Method
dvisc	0.0002652	Paxs	446.93	Joback Method
dvisc	0.0002018	Paxs	484.76	Joback Method
dvisc	0.0001598	Paxs	522.59	Joback Method
dvisc	0.0001306	Paxs	560.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142902&Units=SI
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

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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