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

Inchi: InChI=1S/C12H18O2/c1-5-6-10-11(13-3)7-9(2)8-12(10)14-4/h7-8H,5-6H2,1-4H3
InchiKey: GAZFCNGHTGOHBT-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCCc1c(OC)cc(C)cc1OC
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	1430.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1430.00		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/mol×K	560.42	Joback Method
cpg	468.57	J/mol×K	726.40	Joback Method
cpg	455.88	J/mol×K	693.20	Joback Method
cpg	442.54	J/mol×K	660.01	Joback Method
cpg	428.55	J/mol×K	626.81	Joback Method
cpg	413.94	J/mol×K	593.62	Joback Method
cpg	480.61	J/mol×K	759.59	Joback Method

dvisc	0.0001306	Pa×s	560.42	Joback Method
dvisc	0.0001598	Pa×s	522.59	Joback Method
dvisc	0.0002018	Pa×s	484.76	Joback Method
dvisc	0.0002652	Pa×s	446.93	Joback Method
dvisc	0.0003666	Pa×s	409.10	Joback Method
dvisc	0.0005412	Pa×s	371.27	Joback Method
dvisc	0.0008729	Pa×s	333.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143212&Units=SI

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