Benzene, 1,3-dimethoxy-2-propyl

Inchi: InChI=1S/C11H16O2/c1-4-6-9-10(12-2)7-5-8-11(9)13-3/h5,7-8H,4,6H2,1-3H3
InchiKey: FWIVQKGKHLKKCW-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCCc1c(OC)cccc1OC
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-75.11	kJ/mol	Joback Method
hf	-321.22	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.656		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	532.56	K	Joback Method
tc	733.53	K	Joback Method
tf	309.65	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.48	J/mol×K	532.56	Joback Method
cpg	366.13	J/mol×K	566.05	Joback Method
cpg	380.17	J/mol×K	599.55	Joback Method
cpg	393.58	J/mol×K	633.04	Joback Method
cpg	406.38	J/mol×K	666.54	Joback Method
cpg	418.55	J/mol×K	700.03	Joback Method
cpg	430.10	J/mol×K	733.53	Joback Method
dvisc	0.0011230	Pa×s	309.65	Joback Method

dvisc	0.0006634	Pa×s	346.80	Joback Method
dvisc	0.0004340	Pa×s	383.95	Joback Method
dvisc	0.0003060	Pa×s	421.10	Joback Method
dvisc	0.0002283	Pa×s	458.26	Joback Method
dvisc	0.0001780	Pa×s	495.41	Joback Method
dvisc	0.0001437	Pa×s	532.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142942&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