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

Inchi: InChI=1S/C13H20O2/c1-5-6-7-11-8-9-12(14-3)10(2)13(11)15-4/h8-9H,5-7H2,1-4H3
InchiKey: BKVBXDOCWXBPKU-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCCCc1ccc(OC)c(C)c1OC
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-67.90	kJ/mol	Joback Method
hf	-373.97	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.355		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	583.30	K	Joback Method
tc	779.75	K	Joback Method
tf	344.71	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.62	J/mol×K	583.30	Joback Method
cpg	520.79	J/mol×K	747.01	Joback Method
cpg	507.54	J/mol×K	714.27	Joback Method
cpg	493.59	J/mol×K	681.53	Joback Method
cpg	478.96	J/mol×K	648.78	Joback Method
cpg	463.63	J/mol×K	616.04	Joback Method
cpg	533.34	J/mol×K	779.75	Joback Method
dvisc	0.0001208	Pa×s	583.30	Joback Method

dvisc	0.0001488	Pa×s	543.53	Joback Method
dvisc	0.0001893	Pa×s	503.77	Joback Method
dvisc	0.0002510	Pa×s	464.00	Joback Method
dvisc	0.0003509	Pa×s	424.24	Joback Method
dvisc	0.0005257	Pa×s	384.48	Joback Method
dvisc	0.0008646	Pa×s	344.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142982&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

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