

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/molxK	583.30	Joback Method
cpg	463.63	J/molxK	616.04	Joback Method
cpg	478.96	J/molxK	648.78	Joback Method
cpg	493.59	J/molxK	681.53	Joback Method
cpg	507.54	J/molxK	714.27	Joback Method
cpg	520.79	J/molxK	747.01	Joback Method
cpg	533.34	J/molxK	779.75	Joback Method
dvisc	0.0008646	Paxs	344.71	Joback Method

dvisc	0.0005257	Paxs	384.48	Joback Method
dvisc	0.0003509	Paxs	424.24	Joback Method
dvisc	0.0002510	Paxs	464.00	Joback Method
dvisc	0.0001893	Paxs	503.77	Joback Method
dvisc	0.0001488	Paxs	543.53	Joback Method
dvisc	0.0001208	Paxs	583.30	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/ci9903071
Crippen Method:	https://www.cheméo.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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