

Benzene, 1,3-dimethoxy-2-butyl

Inchi:	InChI=1S/C12H18O2/c1-4-5-7-10-11(13-2)8-6-9-12(10)14-3/h6,8-9H,4-5,7H2,1-3H3
InchiKey:	HKRXKZXKXUTCQU-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCCCc1c(OC)ccc1OC
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-66.69	kJ/mol	Joback Method
hf	-341.86	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	50.73	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.046		Crippen Method
mvol	167.920	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
tb	555.44	K	Joback Method
tc	753.59	K	Joback Method
tf	320.92	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/molxK	555.44	Joback Method
cpg	469.46	J/molxK	720.57	Joback Method
cpg	456.65	J/molxK	687.54	Joback Method
cpg	443.16	J/molxK	654.52	Joback Method
cpg	429.00	J/molxK	621.49	Joback Method
cpg	414.17	J/molxK	588.47	Joback Method
cpg	481.59	J/molxK	753.59	Joback Method
dvisc	0.0001336	Paxs	555.44	Joback Method

dvisc	0.0001666	Paxs	516.35	Joback Method
dvisc	0.0002152	Paxs	477.27	Joback Method
dvisc	0.0002910	Paxs	438.18	Joback Method
dvisc	0.0004176	Paxs	399.09	Joback Method
dvisc	0.0006481	Paxs	360.01	Joback Method
dvisc	0.0011194	Paxs	320.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R142779&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

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