3,1-Butyl-1,2-dimethoxy benzene

Inchi: InChI=1S/C12H18O2/c1-4-5-7-10-8-6-9-11(13-2)12(10)14-3/h6,8-9H,4-5,7H2,1-3H3
InchiKey: TYEIKLOYVMBOAQ-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCCCc1cccc(OC)c1OC
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
mcvol	167.920	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
tb	555.44	K	Joback Method
tc	753.59	K	Joback Method
tf	320.92	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	555.44	Joback Method
cpg	414.17	J/mol×K	588.47	Joback Method
cpg	429.00	J/mol×K	621.49	Joback Method
cpg	443.16	J/mol×K	654.52	Joback Method
cpg	456.65	J/mol×K	687.54	Joback Method
cpg	469.46	J/mol×K	720.57	Joback Method
cpg	481.59	J/mol×K	753.59	Joback Method
dvisc	0.0011194	Pa×s	320.92	Joback Method

dvisc	0.0006481	Pa×s	360.01	Joback Method
dvisc	0.0004176	Pa×s	399.09	Joback Method
dvisc	0.0002910	Pa×s	438.18	Joback Method
dvisc	0.0002152	Pa×s	477.27	Joback Method
dvisc	0.0001666	Pa×s	516.35	Joback Method
dvisc	0.0001336	Pa×s	555.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R404958&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