Benzene, 1-butoxy-4-methoxy-

Inchi: InChI=1S/C11H16O2/c1-3-4-9-13-11-7-5-10(12-2)6-8-11/h5-8H,3-4,9H2,1-2H3
InchiKey: LBDWIFOIHJVJBH-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCCCOc1ccc(OC)cc1
Mol. weight [g/mol]: 180.24
CAS: 20743-95-7

Physical Properties

Property code	Value	Unit	Source
gf	-65.48	kJ/mol	Joback Method
hf	-309.75	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	47.84	kJ/mol	Joback Method
ie	7.74 ± 0.01	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.874		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	527.58	K	Joback Method
tc	727.46	K	Joback Method
tf	297.13	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.33	J/mol×K	527.58	Joback Method
cpg	366.28	J/mol×K	560.89	Joback Method
cpg	380.57	J/mol×K	594.21	Joback Method
cpg	394.19	J/mol×K	627.52	Joback Method
cpg	407.16	J/mol×K	660.83	Joback Method
cpg	419.47	J/mol×K	694.14	Joback Method
cpg	431.13	J/mol×K	727.46	Joback Method
dvisc	0.0014941	Pa×s	297.13	Joback Method

dvisc	0.0008152	Pa×s	335.54	Joback Method
dvisc	0.0005038	Pa×s	373.95	Joback Method
dvisc	0.0003405	Pa×s	412.35	Joback Method
dvisc	0.0002460	Pa×s	450.76	Joback Method
dvisc	0.0001871	Pa×s	489.17	Joback Method
dvisc	0.0001480	Pa×s	527.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20743957&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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