Benzene, 1-butyl-4-methoxy-

Inchi: InChI=1S/C11H16O/c1-3-4-5-10-6-8-11(12-2)9-7-10/h6-9H,3-5H2,1-2H3
InchiKey: PRBLRGZSVKMPDX-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCCCc1ccc(OC)cc1
Mol. weight [g/mol]: 164.24
CAS: 18272-84-9

Physical Properties

Property code	Value	Unit	Source
gf	39.52	kJ/mol	Joback Method
hf	-177.53	kJ/mol	Joback Method
hfus	19.09	kJ/mol	Joback Method
hvap	45.43	kJ/mol	Joback Method
ie	8.20 ± 0.10	eV	NIST Webbook
log10ws	-3.23		Crippen Method
logp	3.038		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	505.16	K	Joback Method
tc	706.73	K	Joback Method
tf	274.90	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.06	J/mol×K	505.16	Joback Method
cpg	395.24	J/mol×K	673.13	Joback Method
cpg	382.80	J/mol×K	639.54	Joback Method
cpg	369.68	J/mol×K	605.94	Joback Method
cpg	355.85	J/mol×K	572.35	Joback Method
cpg	341.32	J/mol×K	538.75	Joback Method
cpg	407.02	J/mol×K	706.73	Joback Method
dvisc	0.0001779	Pa×s	505.16	Joback Method

dvisc	0.0002253	Pa×s	466.78	Joback Method
dvisc	0.0002975	Pa×s	428.41	Joback Method
dvisc	0.0004152	Pa×s	390.03	Joback Method
dvisc	0.0006230	Pa×s	351.65	Joback Method
dvisc	0.0010326	Pa×s	313.28	Joback Method
dvisc	0.0019708	Pa×s	274.90	Joback Method

Sources

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=C18272849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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