Benzene, 1-butyl-2-methyl-

Other names: 1-Butyl-2-methylbenzene
1-Methyl-2-butylbenzene
1-Methyl-2-n-Butylbenzene
Toluene, o-butyl-
Inchi: InChI=1S/C11H16/c1-3-4-8-11-9-6-5-7-10(11)2/h5-7,9H,3-4,8H2,1-2H3
InchiKey: NUJILYKLNKQOOX-UHFFFAOYSA-N
Formula: C11H16
SMILES: CCCCc1ccccc1C
Mol. weight [g/mol]: 148.24
CAS: 1595-11-5

Physical Properties

Property code	Value	Unit	Source
gf	144.52	kJ/mol	Joback Method
hf	-45.31	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.338		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1161.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1395.80		NIST Webbook
tb	482.74	K	Joback Method
tc	685.93	K	Joback Method
tf	252.67	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.77	J/mol×K	482.74	Joback Method

cpg	316.42	J/mol×K	516.60	Joback Method
cpg	331.27	J/mol×K	550.47	Joback Method
cpg	345.33	J/mol×K	584.33	Joback Method
cpg	358.64	J/mol×K	618.20	Joback Method
cpg	371.23	J/mol×K	652.06	Joback Method
cpg	383.12	J/mol×K	685.93	Joback Method
dvisc	0.0025675	Pa×s	252.67	Joback Method
dvisc	0.0012843	Pa×s	291.01	Joback Method
dvisc	0.0007549	Pa×s	329.36	Joback Method
dvisc	0.0004957	Pa×s	367.71	Joback Method
dvisc	0.0003524	Pa×s	406.05	Joback Method
dvisc	0.0002657	Pa×s	444.39	Joback Method
dvisc	0.0002096	Pa×s	482.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44020e+01
Coeff. B	-3.98664e+03
Coeff. C	-7.36700e+01
Temperature range (K), min.	356.12
Temperature range (K), max.	512.22

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1595115&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume