Benzene, 1-butyl-3-methyl-

Other names:	Toluene, m-butyl-
	1-Methyl-3-n-Butylbenzene
	Benzene, 1-methyl-3-butyl-
Inchi:	InChI=1S/C11H16/c1-3-4-7-11-8-5-6-10(2)9-11/h5-6,8-9H,3-4,7H2,1-2H3
InchiKey:	OAPCPUDMDJIBOQ-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCCc1cccc(C)c1
Mol. weight [g/mol]:	148.24
CAS:	1595-04-6

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
ie	8.40 ± 0.10	eV	NIST Webbook
log10ws	-3.59		Crippen Method
logp	3.338		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.70		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1140.70		NIST Webbook
rinpol	1145.70		NIST Webbook
rinpol	1151.50		NIST Webbook
rinpol	1140.60		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1141.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1370.80		NIST Webbook
ripol	1370.80		NIST Webbook
ripol	1371.00		NIST Webbook
tb	471.00 ± 5.00	K	NIST Webbook
tb	478.20	K	NIST Webbook
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	371.23	J/mol×K	652.06	Joback Method
cpg	358.64	J/mol×K	618.20	Joback Method
cpg	345.33	J/mol×K	584.33	Joback Method
cpg	331.27	J/mol×K	550.47	Joback Method
cpg	316.42	J/mol×K	516.60	Joback Method
cpg	383.12	J/mol×K	685.93	Joback Method
dvisc	0.0002096	Pa×s	482.74	Joback Method
dvisc	0.0002657	Pa×s	444.39	Joback Method
dvisc	0.0003524	Pa×s	406.05	Joback Method
dvisc	0.0004957	Pa×s	367.71	Joback Method
dvisc	0.0007549	Pa×s	329.36	Joback Method
dvisc	0.0012843	Pa×s	291.01	Joback Method
dvisc	0.0025675	Pa×s	252.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	470.20	K	101.00	NIST Webbook

Sources

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=C1595046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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