Benzene, (3-methylbutyl)-

Other names:	(3-Methylbutyl)benzene
	1-Phenyl-3-methylbutane
	2-Methyl-4-phenylbutane
	3-Methyl-1-phenylbutane
	Benzene, isopentyl-
	Isoamylbenzene
	Isopentylbenzene
Inchi:	InChI=1S/C11H16/c1-10(2)8-9-11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey:	XNXIYYFOYIUJIW-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CC(C)CCc1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	2049-94-7

Physical Properties

Property code	Value	Unit	Source
gf	151.71	kJ/mol	Joback Method
hf	-39.12	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	53.00	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	3.275		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1094.90		NIST Webbook
rinpol	1098.40		NIST Webbook
rinpol	1112.60		NIST Webbook
rinpol	1118.60		NIST Webbook
rinpol	1125.30		NIST Webbook
rinpol	1094.90		NIST Webbook
rinpol	1098.40		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1107.00		NIST Webbook

rinpol	1119.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	466.00 ± 4.00	K	NIST Webbook
tb	463.15 ± 2.00	K	NIST Webbook
tb	466.00 ± 5.00	K	NIST Webbook
tb	466.00 ± 5.00	K	NIST Webbook
tb	471.00 ± 4.00	K	NIST Webbook
tb	467.00 ± 5.00	K	NIST Webbook
tb	472.10 ± 0.50	K	NIST Webbook
tb	466.00 ± 6.00	K	NIST Webbook
tc	683.92	K	Joback Method
tf	225.15	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.07	J/mol×K	477.32	Joback Method
cpg	373.84	J/mol×K	649.49	Joback Method
cpg	360.78	J/mol×K	615.05	Joback Method
cpg	346.91	J/mol×K	580.62	Joback Method
cpg	332.19	J/mol×K	546.19	Joback Method
cpg	316.59	J/mol×K	511.75	Joback Method
cpg	386.13	J/mol×K	683.92	Joback Method
dvisc	0.0002075	Pa×s	477.32	Joback Method

dvisc	0.0002764	Pa×s	435.29	Joback Method
dvisc	0.0003914	Pa×s	393.26	Joback Method
dvisc	0.0006024	Pa×s	351.24	Joback Method
dvisc	0.0010427	Pa×s	309.21	Joback Method
dvisc	0.0021444	Pa×s	267.18	Joback Method
dvisc	0.0057730	Pa×s	225.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42972e+01
Coeff. B	-3.87260e+03
Coeff. C	-7.19410e+01
Temperature range (K), min.	348.37
Temperature range (K), max.	502.91

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=C2049947&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Diffusion Coefficients of Isobutylbenzene, sec-Butylbenzene, and 3-Methylbutylbenzene in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je400336p

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume