Benzene, (1,1-dimethylpropyl)-

Other names:	(1,1-Dimethylpropyl)benzene
	2-Methyl-2-phenylbutane
	2-Phenyl-2-methylbutane
	2-methylbutan-2-ylbenzene
	Benzene, tert-pentyl-
	benzene, tert-amyl-
	tert-Amylbenzene
	tert-Pentylbenzene
Inchi:	InChI=1S/C11H16/c1-4-11(2,3)10-8-6-5-7-9-10/h5-9H,4H2,1-3H3
InchiKey:	QHTJSSMHBLGUHV-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCC(C)(C)c1ccccc1
Mol. weight [g/mol]:	148.24
CAS:	2049-95-8

Physical Properties

Property code	Value	Unit	Source
gf	156.99	kJ/mol	Joback Method
hf	-42.59	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	52.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-4.15		Aqueous Solubility Prediction Method
logp	3.374		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1086.00		NIST Webbook
rinpol	1069.50		NIST Webbook
rinpol	1085.50		NIST Webbook
rinpol	1093.30		NIST Webbook
rinpol	1065.90		NIST Webbook
rinpol	1065.90		NIST Webbook
rinpol	1065.90		NIST Webbook
rinpol	1065.90		NIST Webbook
rinpol	1069.50		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1070.50		NIST Webbook

rinpol	1070.30		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1062.21		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1079.30		NIST Webbook
rinpol	1072.17		NIST Webbook
rinpol	1077.18		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1089.28		NIST Webbook
rinpol	1094.66		NIST Webbook
rinpol	1098.17		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1080.48		NIST Webbook
rinpol	1102.40		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1340.00		NIST Webbook
tb	474.53	K	Joback Method
tc	690.01	K	Joback Method
tf	242.57	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.58	J/mol×K	474.53	Joback Method
cpg	320.10	J/mol×K	510.44	Joback Method

cpg	336.48	J/mol×K	546.36	Joback Method
cpg	351.76	J/mol×K	582.27	Joback Method
cpg	366.02	J/mol×K	618.19	Joback Method
cpg	379.31	J/mol×K	654.10	Joback Method
cpg	391.69	J/mol×K	690.01	Joback Method
dvisc	0.0056791	Pa×s	242.57	Joback Method
dvisc	0.0022674	Pa×s	281.23	Joback Method
dvisc	0.0011302	Pa×s	319.89	Joback Method
dvisc	0.0006546	Pa×s	358.55	Joback Method
dvisc	0.0004217	Pa×s	397.21	Joback Method
dvisc	0.0002937	Pa×s	435.87	Joback Method
dvisc	0.0002169	Pa×s	474.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40335e+01
Coeff. B	-3.71739e+03
Coeff. C	-7.07020e+01
Temperature range (K), min.	341.14
Temperature range (K), max.	496.91

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2049958&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
Thermochemistry of ionic liquid-catalysed reactions. Isomerisation and transalkylation of tert-alkyl-benzenes. Are these systems ideal?:	https://www.doi.org/10.1016/j.jct.2010.01.006

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

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