

Benzene, 1-methyl-3-(1-methylethyl)-

Other names:	1-Isopropyl-3-methylbenzene 1-METHYL-3-ISOPROPYLBENZENE 1-Methyl-3-(1-methylethyl)-benzene 1-Methyl-3-iso-propylbenzene 3-Isopropyltoluene 3-Methyl-1-isopropylbenzene M-ISOPROPYL TOLUENE M-METHYL CUMENE NSC 73975 m-Cymene m-Cymol m-Isopropyltoluene m-Methylisopropylbenzene meta-Cymene «beta»-Cymene Â«betaÂ»-Cymene
Inchi:	InChI=1S/C10H14/c1-8(2)10-6-4-5-9(3)7-10/h4-8H,1-3H3
InchiKey:	XCYJPXQACVEIOS-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	<chem>Cc1cccc(C(C)C)c1</chem>
Mol. weight [g/mol]:	134.22
CAS:	535-77-3

Physical Properties

Property code	Value	Unit	Source
af	0.2790		KDB
chl	-5857.80 ± 2.20	kJ/mol	NIST Webbook
chl	-5857.30 ± 1.00	kJ/mol	NIST Webbook
gf	133.66	kJ/mol	Joback Method
hcg	5865.55	kJ/mol	KDB
hcn	5558.026	kJ/mol	KDB
hf	-29.31	kJ/mol	KDB
hfl	-78.20 ± 2.10	kJ/mol	NIST Webbook
hfl	-78.70 ± 1.10	kJ/mol	NIST Webbook
hfus	11.79	kJ/mol	Joback Method
hvap	50.00	kJ/mol	NIST Webbook
log10ws	-3.13		Crippen Method

logp	3.118		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	2930.00	kPa	KDB
rinpol	1035.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1027.10		NIST Webbook
rinpol	1016.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1002.80		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	999.00		NIST Webbook

rinpol	1010.00	NIST Webbook
rinpol	1013.00	NIST Webbook
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rinpol	1013.00	NIST Webbook
rinpol	999.00	NIST Webbook
rinpol	1006.60	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1018.00	NIST Webbook
rinpol	1024.00	NIST Webbook
rinpol	1000.30	NIST Webbook
rinpol	1001.80	NIST Webbook
rinpol	1011.90	NIST Webbook
rinpol	1018.50	NIST Webbook
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rinpol	1004.00	NIST Webbook
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rinpol	998.10	NIST Webbook
rinpol	1002.40	NIST Webbook
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rinpol	1006.50	NIST Webbook
rinpol	1028.00	NIST Webbook
rinpol	1005.20	NIST Webbook

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rinpol	1003.40	NIST Webbook
rinpol	1006.35	NIST Webbook
rinpol	1008.12	NIST Webbook
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rinpol	1023.11	NIST Webbook
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ripol	1261.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1244.00		NIST Webbook
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ripol	1313.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1279.00		NIST Webbook
tb	448.30	K	KDB
tc	666.00	K	KDB
tf	209.39 ± 0.02	K	NIST Webbook
tf	209.40 ± 0.01	K	NIST Webbook
tf	209.26 ± 0.20	K	NIST Webbook
tf	209.38 ± 0.02	K	NIST Webbook
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.41	J/mol×K	459.42	Joback Method
cpg	272.52	J/mol×K	494.55	Joback Method
cpg	286.82	J/mol×K	529.69	Joback Method
cpg	300.33	J/mol×K	564.82	Joback Method
cpg	313.10	J/mol×K	599.96	Joback Method
cpg	325.13	J/mol×K	635.09	Joback Method
cpg	336.48	J/mol×K	670.22	Joback Method
dvisc	0.0015637	Paxs	265.24	Joback Method

dvisc	0.0035598	Paxs	226.40	Joback Method
dvisc	0.0008475	Paxs	304.07	Joback Method
dvisc	0.0005277	Paxs	342.91	Joback Method
dvisc	0.0003618	Paxs	381.75	Joback Method
dvisc	0.0002660	Paxs	420.58	Joback Method
dvisc	0.0002060	Paxs	459.42	Joback Method
hvapt	44.70	kJ/mol	400.50	NIST Webbook
rfi	1.49050		298.15	KDB
rho1	861.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43637e+01
Coeff. B	-3.85868e+03
Coeff. C	-5.22790e+01
Temperature range (K), min.	326.41
Temperature range (K), max.	478.55

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.49799e+01
Coeff. B	-8.18442e+03
Coeff. C	-8.65797e+00
Coeff. D	3.71735e-06
Temperature range (K), min.	209.44
Temperature range (K), max.	657.00

Sources

KDB:	https://www.thermo.com/files/research/kdb/mol/mol673.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C535773&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=673
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rho:	Liquid Density
rinp:	Non-polar retention indices
rip:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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