

# Benzene, 1,2-diethyl-4-methyl-

<b>Other names:</b>	1,2-Diethyl-4-methylbenzene 1-Methyl-3,4-diethylbenzene Benzene, 3,4-diethyl-1-methyl
<b>Inchi:</b>	InChI=1S/C11H16/c1-4-10-7-6-9(3)8-11(10)5-2/h6-8H,4-5H2,1-3H3
<b>InchiKey:</b>	MJQJAQGFUBIGIK-UHFFFAOYSA-N
<b>Formula:</b>	C11H16
<b>SMILES:</b>	CCc1ccc(C)cc1CC
<b>Mol. weight [g/mol]:</b>	148.24
<b>CAS:</b>	13732-80-4

## Physical Properties

Property code	Value	Unit	Source
gf	134.89	kJ/mol	Joback Method
hf	-56.78	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	43.68	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.120		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
ripol	1154.20		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1154.20		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1159.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1154.00		NIST Webbook
ripol	1154.90		NIST Webbook
ripol	1153.90		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1384.60		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1384.60		NIST Webbook
ripol	1385.00		NIST Webbook

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ripol	1385.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1435.00		NIST Webbook
ripol	1422.00		NIST Webbook
tb	475.00 ± 4.00	K	NIST Webbook
tc	692.15	K	Joback Method
tf	265.19	K	Joback Method
vc	0.543	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.47	J/mol×K	487.72	Joback Method
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method
cpg	331.23	J/mol×K	555.86	Joback Method
cpg	316.73	J/mol×K	521.79	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
dvisc	0.0002015	Paxs	487.72	Joback Method
dvisc	0.0002500	Paxs	450.63	Joback Method
dvisc	0.0003223	Paxs	413.54	Joback Method
dvisc	0.0004370	Paxs	376.46	Joback Method
dvisc	0.0006331	Paxs	339.37	Joback Method
dvisc	0.0010046	Paxs	302.28	Joback Method
dvisc	0.0018138	Paxs	265.19	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43859e+01
Coeff. B	-3.94529e+03
Coeff. C	-7.28340e+01

Temperature range (K), min.	352.67
Temperature range (K), max.	507.60

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13732804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13732804&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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