Benzene, 1,3-diethyl-5-methyl-

Other names:	1,3-DIETHYL-5-METHYLBENZENE
	1-Methyl-3,5-diethylbenzene
	3,5-Diethyltoluene
	Benzene, 3,5-diethyl-1-methyl
	Toluene, 3,5-diethyl-
Inchi:	InChI=1S/C11H16/c1-4-10-6-9(3)7-11(5-2)8-10/h6-8H,4-5H2,1-3H3
InchiKey:	HILAULICMJUOLK-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCc1cc(C)cc(CC)c1
Mol. weight [g/mol]:	148.24
CAS:	2050-24-0

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	2598.00	kPa	KDB
rinpol	1120.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1150.80		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1129.60		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1129.80		NIST Webbook
rinpol	1130.90		NIST Webbook
rinpol	1130.60		NIST Webbook
rinpol	1120.00		NIST Webbook

rinpol	1130.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1398.00		NIST Webbook
tb	473.85 ± 0.20	K	NIST Webbook
tb	472.00 ± 3.00	K	NIST Webbook
tb	471.00 ± 6.00	K	NIST Webbook
tb	478.20	K	KDB
tc	673.30	K	KDB
tf	199.03 ± 0.20	K	NIST Webbook
tf	199.00	K	KDB
vc	0.551	m3/kmol	KDB
zc	0.2557550		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
cpg	301.47	J/mol×K	487.72	Joback Method
cpg	316.73	J/mol×K	521.79	Joback Method
cpg	331.23	J/mol×K	555.86	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
dvisc	0.0002015	Pa×s	487.72	Joback Method
dvisc	0.0002500	Pa×s	450.63	Joback Method
dvisc	0.0018138	Pa×s	265.19	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0004370	Pa×s	376.46	Joback Method
dvisc	0.0003223	Pa×s	413.54	Joback Method
hvapt	49.60	kJ/mol	390.50	NIST Webbook

rhol	874.66	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48010e+01
Coeff. B	-4.34775e+03
Coeff. C	-4.68740e+01
Temperature range (K), min.	346.44
Temperature range (K), max.	505.04

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.68039e+01
Coeff. B	-7.64368e+03
Coeff. C	-5.98248e+00
Coeff. D	3.56913e-06
Temperature range (K), min.	307.15
Temperature range (K), max.	474.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol694.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2050240&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.cheric.org/research/kdb/hcprop/showprop.php?cmpid=694
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
rhol:	Liquid Density
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
zc:	Critical Compressibility