Benzene, 1,3,5-triethyl-

Other names: 1,3,5-Triethylbenzene
Inchi: InChI=1S/C12H18/c1-4-10-7-11(5-2)9-12(6-3)8-10/h7-9H,4-6H2,1-3H3
InchiKey: WJYMPXJVHNDZHD-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCc1cc(CC)cc(CC)c1
Mol. weight [g/mol]: 162.27
CAS: 102-25-0

Physical Properties

Property code	Value	Unit	Source
af	0.4790		KDB
gf	143.31	kJ/mol	Joback Method
hf	-77.42	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	59.20 ± 0.30	kJ/mol	NIST Webbook
ie	8.32	eV	NIST Webbook
log10ws	-3.88		Crippen Method
logp	3.374		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2435.00 ± 100.00	kPa	NIST Webbook
pc	2340.00	kPa	KDB
rhoc	259.63 ± 10.06	kg/m3	NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1207.00		NIST Webbook

rinpol	1207.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1189.10		NIST Webbook
rinpol	1190.80		NIST Webbook
rinpol	1207.10		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1215.10		NIST Webbook
rinpol	1189.10		NIST Webbook
rinpol	1190.80		NIST Webbook
rinpol	1188.34		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1211.55		NIST Webbook
rinpol	1222.30		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1219.60		NIST Webbook
rinpol	1222.30		NIST Webbook
rinpol	1224.30		NIST Webbook
rinpol	1205.70		NIST Webbook
rinpol	1207.60		NIST Webbook
rinpol	1208.10		NIST Webbook
rinpol	1219.60		NIST Webbook
rinpol	1222.30		NIST Webbook
rinpol	1224.30		NIST Webbook
rinpol	1222.30		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1213.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1476.50		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1456.00		NIST Webbook
tb	488.70 ± 0.50	K	NIST Webbook
tb	482.00 ± 5.00	K	NIST Webbook
tb	488.65 ± 0.30	K	NIST Webbook
tb	488.90 ± 0.60	K	NIST Webbook
tb	489.10	K	NIST Webbook

tb	489.20	K	KDB
tb	488.90 ± 1.50	K	NIST Webbook
tc	682.30	K	KDB
tc	679.00 ± 2.00	K	NIST Webbook
tf	206.73 ± 0.02	K	NIST Webbook
tf	206.71 ± 0.03	K	NIST Webbook
tf	206.71 ± 0.03	K	NIST Webbook
tf	207.00	K	KDB
vc	0.600	m3/kmol	KDB
zc	0.2472820		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.80	J/mol×K	510.60	Joback Method
cpg	419.85	J/mol×K	678.59	Joback Method
cpg	406.73	J/mol×K	644.99	Joback Method
cpg	392.88	J/mol×K	611.39	Joback Method
cpg	378.30	J/mol×K	577.79	Joback Method
cpg	362.94	J/mol×K	544.20	Joback Method
cpg	432.28	J/mol×K	712.18	Joback Method
dvisc	0.0001933	Pa×s	510.60	Joback Method
dvisc	0.0002414	Pa×s	471.58	Joback Method
dvisc	0.0003139	Pa×s	432.55	Joback Method
dvisc	0.0004298	Pa×s	393.53	Joback Method
dvisc	0.0006307	Pa×s	354.51	Joback Method
dvisc	0.0010177	Pa×s	315.48	Joback Method
dvisc	0.0018797	Pa×s	276.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45718e+01
Coeff. B	-4.17246e+03
Coeff. C	-6.98540e+01
Temperature range (K), min.	361.96

Temperature range (K), max.	520.43

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.85038e+01
Coeff. B	-8.78865e+03
Coeff. C	-7.50559e+00
Coeff. D	2.38647e-06
Temperature range (K), min.	368.15
Temperature range (K), max.	682.28

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol704.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102250&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=704
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
rhoc:	Critical 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