Benzene, 1,2,4-triethyl-

Other names: 1,2,4-Triethylbenzene
Inchi: InChI=1S/C12H18/c1-4-10-7-8-11(5-2)12(6-3)9-10/h7-9H,4-6H2,1-3H3
InchiKey: WNLWIOJSURYFIB-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCc1ccc(CC)c(CC)c1
Mol. weight [g/mol]: 162.27
CAS: 877-44-1

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	45.91	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.374		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2340.00	kPa	KDB
rinpol	1223.20		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1225.20		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1206.30		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1230.90		NIST Webbook
rinpol	1206.30		NIST Webbook

ripol	1489.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1501.00		NIST Webbook
tb	494.20	K	NIST Webbook
tb	490.70	K	KDB
tc	684.40	K	KDB
tf	207.00	K	KDB
vc	0.600	m3/kmol	KDB
zc	0.2465240		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.80	J/mol×K	510.60	Joback Method
cpg	362.94	J/mol×K	544.20	Joback Method
cpg	378.30	J/mol×K	577.79	Joback Method
cpg	392.88	J/mol×K	611.39	Joback Method
cpg	406.73	J/mol×K	644.99	Joback Method
cpg	419.85	J/mol×K	678.59	Joback Method
cpg	432.28	J/mol×K	712.18	Joback Method
dvisc	0.0018797	Pa×s	276.46	Joback Method
dvisc	0.0010177	Pa×s	315.48	Joback Method
dvisc	0.0006307	Pa×s	354.51	Joback Method
dvisc	0.0004298	Pa×s	393.53	Joback Method
dvisc	0.0003139	Pa×s	432.55	Joback Method
dvisc	0.0002414	Pa×s	471.58	Joback Method
dvisc	0.0001933	Pa×s	510.60	Joback Method
hvapt	51.20	kJ/mol	405.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	490.70	K	101.00	NIST Webbook
tbrp	372.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47976e+01
Coeff. B	-4.43701e+03
Coeff. C	-5.52640e+01
Temperature range (K), min.	361.05
Temperature range (K), max.	523.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.95166e+01
Coeff. B	-8.09603e+03
Coeff. C	-6.32837e+00
Coeff. D	3.27175e-06
Temperature range (K), min.	319.15
Temperature range (K), max.	511.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=703

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/mol703.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C877441&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

Latest version available from:
https://www.chemeo.com/cid/14-610-8/Benzene-1-2-4-triethyl.pdf
Generated by Cheméo on 2024-12-10 02:58:55.471899663 +0000 UTC m=+8380398.108868912.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.