Benzene, 1,3,5-tris(1,1-dimethylethyl)-

Other names:	1,3,5-Tri-t-butylbenzene
	1,3,5-Tris-(1,1-dimethylethyl)benzene
	1,3,5-tri-tert-butylbenzene
	1,3,5-tris(tert-butyl)benzene
Inchi:	InChI=1S/C18H30/c1-16(2,3)13-10-14(17(4,5)6)12-15(11-13)18(7,8)9/h10-12H,1-9H3
InchiKey:	GUFMBISUSZUUCB-UHFFFAOYSA-N
Formula:	C18H30
SMILES:	CC(C)(C)c1cc(C(C)(C)C)cc(C(C)(C)C)c1
Mol. weight [g/mol]:	246.44
CAS:	1460-02-2

Physical Properties

Property code	Value	Unit	Source
af	0.4976		Cheméo Relay (1.0)
affp	848.80	kJ/mol	NIST Webbook
basg	822.30	kJ/mol	NIST Webbook
chs	-11049.00 ± 4.00	kJ/mol	NIST Webbook
hf	-215.70	kJ/mol	Cheméo Relay (1.0)
hfl	-306.80 ± 2.30	kJ/mol	NIST Webbook
hfus	13.40	kJ/mol	Joback Method
hsub	79.70 ± 0.40	kJ/mol	NIST Webbook
hsub	81.20 ± 0.30	kJ/mol	NIST Webbook
hvap	69.87	kJ/mol	Cheméo Relay (1.0)
ie	8.46	eV	NIST Webbook
ie	8.19	eV	NIST Webbook
ie	8.56 ± 0.07	eV	NIST Webbook
log10ws	-7.04		Cheméo Relay (1.0)
logp	5.579		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
tb	521.20	K	NIST Webbook
tc	757.78	K	Cheméo Relay (1.0)
tf	346.30 ± 0.50	K	NIST Webbook
tf	346.80 ± 0.70	K	NIST Webbook
tf	345.05 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.94	J/mol×K	856.65	Joback Method
cpg	683.70	J/mol×K	674.60	Joback Method
cpg	704.32	J/mol×K	711.01	Joback Method
cpg	661.58	J/mol×K	638.19	Joback Method
cpg	723.53	J/mol×K	747.42	Joback Method
cpg	741.47	J/mol×K	783.83	Joback Method
cpg	758.23	J/mol×K	820.24	Joback Method
dvisc	0.0001639	Pa×s	542.57	Joback Method
dvisc	0.0023578	Pa×s	351.34	Joback Method
dvisc	0.0009528	Pa×s	399.15	Joback Method
dvisc	0.0004674	Pa×s	446.96	Joback Method
dvisc	0.0002631	Pa×s	494.77	Joback Method
dvisc	0.0001102	Pa×s	590.38	Joback Method
dvisc	0.0000787	Pa×s	638.19	Joback Method
hsubt	79.90 ± 0.30	kJ/mol	319.50	NIST Webbook
hsubt	79.70 ± 0.40	kJ/mol	294.00	NIST Webbook
pvap	0.33	kPa	367.45	Study and prediction of alkylbenzenes vapour pressures
pvap	0.26	kPa	363.45	Study and prediction of alkylbenzenes vapour pressures
pvap	0.63	kPa	379.55	Study and prediction of alkylbenzenes vapour pressures
pvap	0.57	kPa	377.35	Study and prediction of alkylbenzenes vapour pressures
pvap	0.49	kPa	374.95	Study and prediction of alkylbenzenes vapour pressures
pvap	0.44	kPa	372.65	Study and prediction of alkylbenzenes vapour pressures
pvap	0.13	kPa	352.15	Study and prediction of alkylbenzenes vapour pressures

pvap	0.38	kPa	370.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.29	kPa	365.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.74	kPa	382.65	Study and prediction of alkylbenzenes vapour pressures
pvap	0.24	kPa	362.05	Study and prediction of alkylbenzenes vapour pressures
pvap	0.23	kPa	361.35	Study and prediction of alkylbenzenes vapour pressures
pvap	0.20	kPa	359.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.20	kPa	358.95	Study and prediction of alkylbenzenes vapour pressures
pvap	0.18	kPa	356.65	Study and prediction of alkylbenzenes vapour pressures
pvap	0.15	kPa	354.45	Study and prediction of alkylbenzenes vapour pressures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.70	K	1.60	NIST Webbook
tbrp	402.00 ± 1.00	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.10369e+01
Coeff. B	-3.28329e+03
Coeff. C	-8.60570e+01
Temperature range (K), min.	391.15
Temperature range (K), max.	659.15

Sources

Cheméo Relay (1.0):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460022&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

Study and prediction of alkylbenzenes vapour pressures: https://www.doi.org/10.1016/j.fluid.2008.04.016

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

Cheméo Relay (1.0, beta):

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point