Benzene, 1,3-bis(1,1-dimethylethyl)-5-methyl-

Other names:	1,3-Ditert-butyl-5-methylbenzene
	1,3-bis(1,1-dimethylethyl)-5-methylbenzene
	1,3-di-(t-C4H9)-5-CH3-C6H3
	1,3-di-tert-butyl-5-methylbenzene
	3,5-Di-tert-butyltoluene
	3,5-bis(tert-butyl)toluene
	Benzene, 1-methyl-3,5-bis-(1,1-dimethylethyl)
	Benzene, 1-methyl-3,5-bis-(tert-butyl)
	Toluene, 3,5-di-tert-butyl-
Inchi:	InChI=1S/C15H24/c1-11-8-12(14(2,3)4)10-13(9-11)15(5,6)7/h8-10H,1-7H3
InchiKey:	WIXDSJRJFDWTNY-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	Cc1cc(C(C)(C)C)cc(C(C)(C)C)c1
Mol. weight [g/mol]:	204.35
CAS:	15181-11-0

Physical Properties

Property code	Value	Unit	Source
affp	853.70	kJ/mol	NIST Webbook
basg	826.00	kJ/mol	NIST Webbook
gf	174.25	kJ/mol	Joback Method
hf	-156.84	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hsub	81.80 ± 0.50	kJ/mol	NIST Webbook
hvap	63.30 ± 0.90	kJ/mol	NIST Webbook
log10ws	-4.57		Crippen Method
logp	4.590		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1507.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1732.00		NIST Webbook
tb	517.20	K	NIST Webbook
tc	789.98	K	Joback Method
tf	304.30 ± 1.00	K	NIST Webbook
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.04	J/mol×K	789.98	Joback Method
cpg	519.60	J/mol×K	608.98	Joback Method
cpg	538.63	J/mol×K	645.18	Joback Method
cpg	556.41	J/mol×K	681.38	Joback Method
cpg	573.01	J/mol×K	717.58	Joback Method
cpg	588.53	J/mol×K	753.78	Joback Method
cpg	499.24	J/mol×K	572.78	Joback Method
dvisc	0.0001765	Pa×s	529.84	Joback Method
dvisc	0.0002519	Pa×s	486.89	Joback Method
dvisc	0.0003850	Pa×s	443.94	Joback Method
dvisc	0.0006443	Pa×s	401.00	Joback Method
dvisc	0.0012201	Pa×s	358.06	Joback Method
dvisc	0.0001305	Pa×s	572.78	Joback Method
dvisc	0.0027496	Pa×s	315.11	Joback Method
hsubt	82.40 ± 0.50	kJ/mol	288.00	NIST Webbook
hvapt	61.80 ± 0.90	kJ/mol	323.50	NIST Webbook
pvap	0.04	kPa	320.45	Study and prediction of alkylbenzenes vapour pressures
pvap	0.07	kPa	327.95	Study and prediction of alkylbenzenes vapour pressures
pvap	0.03	kPa	317.95	Study and prediction of alkylbenzenes vapour pressures
pvap	0.10	kPa	333.05	Study and prediction of alkylbenzenes vapour pressures
pvap	0.11	kPa	335.55	Study and prediction of alkylbenzenes vapour pressures
pvap	0.13	kPa	338.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.15	kPa	340.65	Study and prediction of alkylbenzenes vapour pressures

pvap	0.18	kPa	343.05	Study and prediction of alkylbenzenes vapour pressures
pvap	0.21	kPa	345.55	Study and prediction of alkylbenzenes vapour pressures
pvap	0.25	kPa	348.10	Study and prediction of alkylbenzenes vapour pressures
pvap	0.28	kPa	350.45	Study and prediction of alkylbenzenes vapour pressures
pvap	0.33	kPa	353.05	Study and prediction of alkylbenzenes vapour pressures
pvap	0.37	kPa	355.65	Study and prediction of alkylbenzenes vapour pressures
pvap	0.44	kPa	358.15	Study and prediction of alkylbenzenes vapour pressures
pvap	0.03	kPa	315.45	Study and prediction of alkylbenzenes vapour pressures
pvap	0.02	kPa	313.35	Study and prediction of alkylbenzenes vapour pressures
pvap	0.02	kPa	310.65	Study and prediction of alkylbenzenes vapour pressures
pvap	0.02	kPa	308.25	Study and prediction of alkylbenzenes vapour pressures
pvap	0.06	kPa	325.55	Study and prediction of alkylbenzenes vapour pressures
pvap	0.05	kPa	323.05	Study and prediction of alkylbenzenes vapour pressures
pvap	0.08	kPa	330.55	Study and prediction of alkylbenzenes vapour pressures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48062e+01
Coeff. B	-4.40352e+03
Coeff. C	-8.49180e+01
Temperature range (K), min.	388.22
Temperature range (K), max.	548.70

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15181110&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Study and prediction of alkylbenzenes vapour pressures:	https://www.doi.org/10.1016/j.fluid.2008.04.016

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume