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

Other names:	1,3,5-Triisopropylbenzene
	2,4,6-Triisopropylbenzene
	Benzene, 1,3,5-triisopropyl-
Inchi:	InChI=1S/C15H24/c1-10(2)13-7-14(11(3)4)9-15(8-13)12(5)6/h7-12H,1-6H3
InchiKey:	VUMCUSHVMYIRMB-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC(C)c1cc(C(C)C)cc(C(C)C)c1
Mol. weight [g/mol]:	204.35
CAS:	717-74-8

Physical Properties

Property code	Value	Unit	Source
gf	161.25	kJ/mol	Joback Method
hf	-155.18	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	64.60 ± 0.60	kJ/mol	NIST Webbook
ie	8.24	eV	NIST Webbook
log10ws	-5.03		Crippen Method
logp	5.057		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1322.60		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1285.70		NIST Webbook
rinpol	1287.50		NIST Webbook
rinpol	1324.90		NIST Webbook
rinpol	1325.70		NIST Webbook
rinpol	1326.70		NIST Webbook
rinpol	1285.70		NIST Webbook
rinpol	1287.50		NIST Webbook
rinpol	1282.82		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1324.30		NIST Webbook
rinpol	1322.60		NIST Webbook

rinpol	1322.80		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1326.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1457.80		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1457.80		NIST Webbook
ripol	1495.20		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	509.40 ± 1.00	K	NIST Webbook
tb	511.20	K	NIST Webbook
tb	507.20	K	NIST Webbook
tc	783.37	K	Joback Method
tf	265.80 ± 1.00	K	NIST Webbook
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.44	J/mol×K	577.92	Joback Method
cpg	513.86	J/mol×K	612.16	Joback Method
cpg	532.26	J/mol×K	646.40	Joback Method
cpg	549.66	J/mol×K	680.65	Joback Method
cpg	566.10	J/mol×K	714.89	Joback Method
cpg	581.61	J/mol×K	749.13	Joback Method
cpg	596.23	J/mol×K	783.37	Joback Method
dvisc	0.0016012	Pa×s	317.38	Joback Method
dvisc	0.0047804	Pa×s	265.27	Joback Method
dvisc	0.0007301	Pa×s	369.49	Joback Method
dvisc	0.0004043	Pa×s	421.59	Joback Method
dvisc	0.0002549	Pa×s	473.70	Joback Method
dvisc	0.0001761	Pa×s	525.81	Joback Method

dvisc	0.0001301	Pa×s	577.92	Joback Method
hvapt	64.30 ± 0.30	kJ/mol	303.00	NIST Webbook
hvapt	67.40	kJ/mol	335.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51205e+01
Coeff. B	-4.45239e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	383.42
Temperature range (K), max.	537.16

Sources

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
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=C717748&Units=SI

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
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
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

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