

Benzene, 1,2-bis(1-methylethyl)-

Other names:	1,2-DIISOPROPYLBENZENE 1,2-bis(1-methylethyl)benzene Benzene, 1,2-di-(1-methylethyl) Benzene, o-diisopropyl- o-Diisopropylbenzene
Inchi:	InChI=1S/C12H18/c1-9(2)11-7-5-6-8-12(11)10(3)4/h5-10H,1-4H3
InchiKey:	OKIRBHVFGXOIS-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CC(C)c1ccccc1C(C)C
Mol. weight [g/mol]:	162.27
CAS:	577-55-9

Physical Properties

Property code	Value	Unit	Source
gf	148.06	kJ/mol	Joback Method
hf	-76.51	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	44.47	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.933		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2446.00	kPa	KDB
rinpol	1118.10		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1153.05		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1120.30		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1162.20		NIST Webbook
rinpol	1118.10		NIST Webbook

ripol	1120.30		NIST Webbook
ripol	1152.40		NIST Webbook
ripol	1157.20		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1378.00		NIST Webbook
tb	477.00 ± 3.00	K	NIST Webbook
tb	476.90 ± 10.00	K	NIST Webbook
tb	447.15	K	KDB
tc	668.95	K	KDB
tf	216.49	K	KDB
tf	216.47 ± 4.00	K	NIST Webbook
vc	0.583	m3/kmol	KDB
zc	0.2563420		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.53	J/molxK	679.35	Joback Method
cpg	437.55	J/molxK	714.27	Joback Method
cpg	346.60	J/molxK	504.74	Joback Method
cpg	364.01	J/molxK	539.66	Joback Method
cpg	380.47	J/molxK	574.58	Joback Method
cpg	396.02	J/molxK	609.51	Joback Method
cpg	410.70	J/molxK	644.43	Joback Method
dvisc	0.0001786	Paxs	504.74	Joback Method
dvisc	0.0002390	Paxs	459.61	Joback Method
dvisc	0.0055461	Paxs	233.94	Joback Method
dvisc	0.0019687	Paxs	279.07	Joback Method
dvisc	0.0009324	Paxs	324.21	Joback Method
dvisc	0.0005301	Paxs	369.34	Joback Method
dvisc	0.0003408	Paxs	414.47	Joback Method
hvapt	48.90	kJ/mol	432.00	NIST Webbook
rho1	876.28	kg/m3	293.10	KDB

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32128e+01
Coeff. B	-3.27062e+03
Coeff. C	-9.65990e+01
Temperature range (K), min.	349.64
Temperature range (K), max.	510.53

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.16259e+02
Coeff. B	-1.08049e+04
Coeff. C	-1.47083e+01
Coeff. D	7.59221e-06
Temperature range (K), min.	388.15
Temperature range (K), max.	476.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577559&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.thermo.com/research/kdb/hcprop/showprop.php?cmpid=699
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol699.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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