

Benzene, 1-methyl-2-(2-propenyl)-

Other names:	Toluene, o-allyl- o-Allyltoluene 1-Allyl-2-methylbenzene 2-Allyl-1-methylbenzene 2-Allyltoluene 1-Methyl-2-(2-propenyl)benzene
Inchi:	InChI=1S/C10H12/c1-3-6-10-8-5-4-7-9(10)2/h3-5,7-8H,1,6H2,2H3
InchiKey:	SVIHJJUMPAUQNO-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=CCc1ccccc1C
Mol. weight [g/mol]:	132.20
CAS:	1587-04-8

Physical Properties

Property code	Value	Unit	Source
gf	223.94	kJ/mol	Joback Method
hf	100.76	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
ie	7.78 ± 0.04	eV	NIST Webbook
log10ws	-3.02		Crippen Method
logp	2.724		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1004.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1442.00		NIST Webbook
tb	448.00 ± 4.00	K	NIST Webbook
tc	667.08	K	Joback Method
tf	239.64	K	Joback Method

vc

0.469

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.59	J/mol×K	456.54	Joback Method
cpg	254.60	J/mol×K	491.63	Joback Method
cpg	267.82	J/mol×K	526.72	Joback Method
cpg	280.28	J/mol×K	561.81	Joback Method
cpg	292.01	J/mol×K	596.90	Joback Method
cpg	303.05	J/mol×K	631.99	Joback Method
cpg	313.43	J/mol×K	667.08	Joback Method
dvisc	0.0021934	Paxs	239.64	Joback Method
dvisc	0.0011572	Paxs	275.79	Joback Method
dvisc	0.0007081	Paxs	311.94	Joback Method
dvisc	0.0004798	Paxs	348.09	Joback Method
dvisc	0.0003498	Paxs	384.24	Joback Method
dvisc	0.0002693	Paxs	420.39	Joback Method
dvisc	0.0002161	Paxs	456.54	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1587048&Units=SI>

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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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