Benzene, 1-methyl-4-(2-propenyl)-

Other names:	p-Allyltoluene
	p-Methylallylbenzene
	Toluene, p-allyl-
	1-Allyl-4-methylbenzene
	3-p-Tolylpropene
	4-Allyltoluene
	1-Methyl-4-(2-propenyl)benzene
	1-Methyl-4-allylbenzene
Inchi:	InChI=1S/C10H12/c1-3-4-10-7-5-9(2)6-8-10/h3,5-8H,1,4H2,2H3
InchiKey:	WAEOXIOXMKNFLQ-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=CCc1ccc(C)cc1
Mol. weight [g/mol]:	132.20
CAS:	3333-13-9

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
log10ws	-3.02		Crippen Method
logp	2.724		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1047.00		NIST Webbook
rinpol	180.40		NIST Webbook
rinpol	1033.30		NIST Webbook
rinpol	1033.30		NIST Webbook
rinpol	1033.00		NIST Webbook
tb	459.00 ± 5.00	K	NIST Webbook
tb	456.13 ± 0.30	K	NIST Webbook
tb	456.06 ± 0.30	K	NIST Webbook
tb	456.06 ± 0.50	K	NIST Webbook
tc	667.08	K	Joback Method
tf	228.28 ± 0.30	K	NIST Webbook
tf	228.44 ± 0.20	K	NIST Webbook

tf	228.44 ± 0.50	K	NIST Webbook
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	303.05	J/mol×K	631.99	Joback Method
cpg	292.01	J/mol×K	596.90	Joback Method
cpg	280.28	J/mol×K	561.81	Joback Method
cpg	267.82	J/mol×K	526.72	Joback Method
cpg	254.60	J/mol×K	491.63	Joback Method
cpg	313.43	J/mol×K	667.08	Joback Method
dvisc	0.0002161	Pa×s	456.54	Joback Method
dvisc	0.0002693	Pa×s	420.39	Joback Method
dvisc	0.0003498	Pa×s	384.24	Joback Method
dvisc	0.0004798	Pa×s	348.09	Joback Method
dvisc	0.0007081	Pa×s	311.94	Joback Method
dvisc	0.0011572	Pa×s	275.79	Joback Method
dvisc	0.0021934	Pa×s	239.64	Joback Method

Sources

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=C3333139&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume