

1-Allyl-4-methylbenzene

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]:	132.21

Physical Properties

Property code	Value	Unit	Source
af	0.3307		Cheméo Relay (1.0)
gf	223.94	kJ/mol	Joback Method
hf	112.29	kJ/mol	Cheméo Relay (1.0)
hfus	14.03	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-3.29		Cheméo Relay (1.0)
logp	2.724		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1033.30		NIST Webbook
rinpol	1033.30		NIST Webbook
rinpol	180.40		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	180.40		NIST Webbook
rinpol	1047.00		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
tb	459.00 ± 5.00	K	NIST Webbook
tc	649.94	K	Cheméo Relay (1.0)

tf	228.44 ± 0.50	K	NIST Webbook
tf	228.44 ± 0.20	K	NIST Webbook
tf	228.28 ± 0.30	K	NIST Webbook
vc	0.454	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.59	J/mol×K	456.54	Joback Method
cpg	313.43	J/mol×K	667.08	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
dvisc	0.0004798	Pa×s	348.09	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	0.0021934	Pa×s	239.64	Joback Method
dvisc	0.0007081	Pa×s	311.94	Joback Method
dvisc	0.0011572	Pa×s	275.79	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3333139&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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