Benzene, 1-methyl-4-(1,1-dimethylpropyl)

Other names:	1-(1,1-dimethylpropyl)-4-methylbenzene 1-methyl-4-tert-pentylbenzene benzene, 1-(1,1-dimethylpropyl)-4-methyl- p-tert-amyltoluene toluene, p-tert-pentyl-
Inchi:	InChI=1S/C12H18/c1-5-12(3,4)11-8-6-10(2)7-9-11/h6-9H,5H2,1-4H3
InchiKey:	HTICYVWLHLMMPF-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCC(C)(C)c1ccc(C)cc1
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	155.78	kJ/mol	Joback Method
hf	-74.70	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.683		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1192.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1411.00		NIST Webbook
tb	502.39	K	Joback Method
tc	715.84	K	Joback Method
tf	266.36	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.05	J/mol×K	502.39	Joback Method
cpg	366.88	J/mol×K	537.97	Joback Method
cpg	383.61	J/mol×K	573.54	Joback Method
cpg	399.29	J/mol×K	609.12	Joback Method
cpg	413.98	J/mol×K	644.69	Joback Method
cpg	427.73	J/mol×K	680.27	Joback Method
cpg	440.60	J/mol×K	715.84	Joback Method
dvisc	0.0036209	Pa×s	266.36	Joback Method
dvisc	0.0016213	Pa×s	305.70	Joback Method
dvisc	0.0008720	Pa×s	345.04	Joback Method
dvisc	0.0005324	Pa×s	384.38	Joback Method
dvisc	0.0003563	Pa×s	423.71	Joback Method
dvisc	0.0002553	Pa×s	463.05	Joback Method
dvisc	0.0001927	Pa×s	502.39	Joback Method

Sources

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=R525694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of ionic liquid-catalysed reactions. Isomerisation and transalkylation of tert-alkyl-benzenes. Are these systems ideal?:	https://www.doi.org/10.1016/j.jct.2010.01.006

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume