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

Other names: Toluene, p-isobutyl-
Inchi: InChI=1S/C11H16/c1-9(2)8-11-6-4-10(3)5-7-11/h4-7,9H,8H2,1-3H3
InchiKey: VCGBZXLLPCGFQM-UHFFFAOYSA-N
Formula: C11H16
SMILES: Cc1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 148.24
CAS: 5161-04-6

Physical Properties

Property code	Value	Unit	Source
gf	142.08	kJ/mol	Joback Method
hf	-50.59	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.194		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	470.00 ± 6.00	K	NIST Webbook
tc	690.17	K	Joback Method
tf	237.67	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.93	J/mol×K	482.30	Joback Method
cpg	373.16	J/mol×K	655.52	Joback Method
cpg	360.30	J/mol×K	620.88	Joback Method
cpg	346.68	J/mol×K	586.23	Joback Method
cpg	332.27	J/mol×K	551.59	Joback Method
cpg	317.03	J/mol×K	516.94	Joback Method
cpg	385.28	J/mol×K	690.17	Joback Method
dvisc	0.0001987	Pa×s	482.30	Joback Method

dvisc	0.0002582	Pa×s	441.53	Joback Method
dvisc	0.0003537	Pa×s	400.76	Joback Method
dvisc	0.0005204	Pa×s	359.99	Joback Method
dvisc	0.0008449	Pa×s	319.21	Joback Method
dvisc	0.0015812	Pa×s	278.44	Joback Method
dvisc	0.0036688	Pa×s	237.67	Joback Method

Sources

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=C5161046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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