1-Methyl-2-isobutylbenzene

Other names: Benzene, 1-methyl-2-(2-methylpropyl)-
o-isobutyltoluene
2-isobutyltoluene
Inchi: InChI=1S/C11H16/c1-9(2)8-11-7-5-4-6-10(11)3/h4-7,9H,8H2,1-3H3
InchiKey: XNMPJDZAHSMAMN-UHFFFAOYSA-N
Formula: C11H16
SMILES: Cc1ccccc1CC(C)C
Mol. weight [g/mol]: 148.24
CAS: 36301-29-8

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
rinpol	1027.85		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1331.60		NIST Webbook
tb	482.30	K	Joback Method
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: 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=C36301298&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume