

Benzene, 1-methyl-3-(1-methylpropyl)

Other names:	1-sec-butyl-3-methylbenzene
Inchi:	InChI=1S/C11H16/c1-4-10(3)11-7-5-6-9(2)8-11/h5-8,10H,4H2,1-3H3
InchiKey:	RMNILBOMCXQZFC-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCC(C)c1cccc(C)c1
Mol. weight [g/mol]:	148.24
CAS:	1772-10-7

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	-3.55		Crippen Method
logp	3.509		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
tb	469.00 ± 6.00	K	NIST Webbook
tb	468.00 ± 5.00	K	NIST Webbook
tc	690.17	K	Joback Method
tf	237.67	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.93	J/mol×K	482.30	Joback Method
cpg	317.03	J/mol×K	516.94	Joback Method
cpg	332.27	J/mol×K	551.59	Joback Method

cpg	346.68	J/molxK	586.23	Joback Method
cpg	360.30	J/molxK	620.88	Joback Method
cpg	373.16	J/molxK	655.52	Joback Method
cpg	385.28	J/molxK	690.17	Joback Method
dvisc	0.0036688	Paxs	237.67	Joback Method
dvisc	0.0015812	Paxs	278.44	Joback Method
dvisc	0.0008449	Paxs	319.21	Joback Method
dvisc	0.0005204	Paxs	359.99	Joback Method
dvisc	0.0003537	Paxs	400.76	Joback Method
dvisc	0.0002582	Paxs	441.53	Joback Method
dvisc	0.0001987	Paxs	482.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1772107&Units=SI
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

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

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