Benzene, 1-methyl-3-(2-methylpropyl)-

Other names: 1-methyl-3-(2-methylpropy)benzene
Benzene, 1-methyl-3-(2-methylpropyl)-
Benzene, 1-methyl-3-isobutyl
Inchi: InChI=1S/C11H16/c1-9(2)7-11-6-4-5-10(3)8-11/h4-6,8-9H,7H2,1-3H3
InchiKey: SDHYGAUOCHFYSR-UHFFFAOYSA-N
Formula: C11H16
SMILES: Cc1cccc(CC(C)C)c1
Mol. weight [g/mol]: 148.25

Physical Properties

Property code	Value	Unit	Source
af	0.4074		Cheméo Relay (1.0)
gf	142.08	kJ/mol	Joback Method
hf	-57.23	kJ/mol	Cheméo Relay (1.0)
hfus	14.37	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.194		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
ripol	1309.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1308.90		NIST Webbook
ripol	1309.00		NIST Webbook
tb	469.58	K	Cheméo Relay (1.0)
tc	665.23	K	Cheméo Relay (1.0)
tf	206.98	K	Cheméo Relay (1.0)
vc	0.531	m3/kmol	Cheméo Relay (1.0)

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/mol×K	586.23	Joback Method
cpg	360.30	J/mol×K	620.88	Joback Method
cpg	373.16	J/mol×K	655.52	Joback Method
cpg	385.28	J/mol×K	690.17	Joback Method
dvisc	0.0036688	Pa×s	237.67	Joback Method
dvisc	0.0015812	Pa×s	278.44	Joback Method
dvisc	0.0008449	Pa×s	319.21	Joback Method
dvisc	0.0005204	Pa×s	359.99	Joback Method
dvisc	0.0003537	Pa×s	400.76	Joback Method
dvisc	0.0002582	Pa×s	441.53	Joback Method
dvisc	0.0001987	Pa×s	482.30	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5160996&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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