1-Isopropyl-2,3-dimethylbenzene

Other names:	1,2-Dimethyl-3-isopropylbenzene
	Benzene, 1,2-dimethyl-3-(1-methylethyl)-
Inchi:	InChI=1S/C11H16/c1-8(2)11-7-5-6-9(3)10(11)4/h5-8H,1-4H3
InchiKey:	GDEQPEBFOWYWSA-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1cccc(C(C)C)c1C
Mol. weight [g/mol]:	148.24
CAS:	22539-65-7

Physical Properties

Property code	Value	Unit	Source
gf	132.45	kJ/mol	Joback Method
hf	-62.06	kJ/mol	Joback Method
hfus	13.99	kJ/mol	Joback Method
hvap	43.29	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.427		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1134.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1440.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1481.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1454.00		NIST Webbook
tb	477.70 ± 1.00	K	NIST Webbook
tc	696.41	K	Joback Method
tf	250.19	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.65	J/mol×K	487.28	Joback Method
cpg	317.34	J/mol×K	522.13	Joback Method
cpg	332.23	J/mol×K	556.99	Joback Method
cpg	346.36	J/mol×K	591.84	Joback Method
cpg	359.74	J/mol×K	626.70	Joback Method
cpg	372.40	J/mol×K	661.55	Joback Method
cpg	384.36	J/mol×K	696.41	Joback Method
dvisc	0.0024629	Pa×s	250.19	Joback Method
dvisc	0.0012026	Pa×s	289.70	Joback Method
dvisc	0.0006975	Pa×s	329.22	Joback Method
dvisc	0.0004546	Pa×s	368.74	Joback Method
dvisc	0.0003219	Pa×s	408.25	Joback Method
dvisc	0.0002423	Pa×s	447.76	Joback Method
dvisc	0.0001909	Pa×s	487.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42580e+01
Coeff. B	-3.88582e+03
Coeff. C	-7.26440e+01
Temperature range (K), min.	350.79
Temperature range (K), max.	506.98

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22539657&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

KDB:	https://www.cheric.org/files/research/kdb/mol/mol691.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
pvap:	Vapor 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