4-isopropyl-1,2-dimethyl-benzene

Other names:	1,2-Dimethyl-4-isopropylbenzene
	Benzene, 1,2-dimethyl-4-isopropyl
Inchi:	InChI=1S/C11H16/c1-8(2)11-6-5-9(3)10(4)7-11/h5-8H,1-4H3
InchiKey:	MGMSKQZIAGFMRU-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1ccc(C(C)C)cc1C
Mol. weight [g/mol]:	148.25
CAS:	4132-77-8

Physical Properties

Property code	Value	Unit	Source
af	0.3923		Cheméo Relay (1.0)
gf	132.45	kJ/mol	Joback Method
hf	-59.59	kJ/mol	Cheméo Relay (1.0)
hfus	13.99	kJ/mol	Joback Method
hvap	55.61	kJ/mol	Cheméo Relay (1.0)
ie	8.18	eV	Cheméo Relay (1.0)
log10ws	-4.36		Cheméo Relay (1.0)
logp	3.427		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1117.50		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1372.50		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1450.00		NIST Webbook
ripol	1435.00		NIST Webbook

ripol	1423.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1411.00		NIST Webbook
tb	473.00 ± 5.00	K	NIST Webbook
tc	681.94	K	Cheméo Relay (1.0)
tf	247.69	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	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	447.77	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	1.42585e+01
Coeff. B	-3.87977e+03
Coeff. C	-7.24920e+01
Temperature range (K), min.	350.20
Temperature range (K), max.	506.13

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4132778&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

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
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