1,2-Dimethyl-3-propylbenzene

Other names:	1,2-Di-Methyl-3-n-Propylbenzene
	Benzene, 1,2-dimethyl-3-propyl
Inchi:	InChI=1S/C11H16/c1-4-6-11-8-5-7-9(2)10(11)3/h5,7-8H,4,6H2,1-3H3
InchiKey:	IRUSTUOJENXLMN-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCc1cccc(C)c1C
Mol. weight [g/mol]:	148.24
CAS:	17059-44-8

Physical Properties

Property code	Value	Unit	Source
gf	134.89	kJ/mol	Joback Method
hf	-56.78	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	43.68	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.256		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1188.00		NIST Webbook
tb	487.72	K	Joback Method
tc	692.15	K	Joback Method
tf	265.19	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.47	J/mol×K	487.72	Joback Method
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method

cpg	331.23	J/mol×K	555.86	Joback Method
cpg	316.73	J/mol×K	521.79	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
dvisc	0.0002015	Pa×s	487.72	Joback Method
dvisc	0.0002500	Pa×s	450.63	Joback Method
dvisc	0.0003223	Pa×s	413.54	Joback Method
dvisc	0.0004370	Pa×s	376.46	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method
dvisc	0.0018138	Pa×s	265.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43817e+01
Coeff. B	-3.99974e+03
Coeff. C	-7.41830e+01
Temperature range (K), min.	357.97
Temperature range (K), max.	515.16

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42817&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/mol690.mol

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