1,3-Dimethyl-2-propylbenzene

Other names:	1,3-Dimethyl-2-n-Propylbenzene
	Benzene, 1,3-dimethyl-2-propyl-
	m-xylene, 2-propyl-
Inchi:	InChI=1S/C11H16/c1-4-6-11-9(2)7-5-8-10(11)3/h5,7-8H,4,6H2,1-3H3
InchiKey:	POVRSTNZQPBWAS-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCc1c(C)cccc1C
Mol. weight [g/mol]:	148.24
CAS:	17059-45-9

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	1160.00		NIST Webbook
ripol	1451.60		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1452.00		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	316.73	J/mol×K	521.79	Joback Method

cpg	331.23	J/mol×K	555.86	Joback Method
cpg	345.01	J/mol×K	589.93	Joback Method
cpg	358.09	J/mol×K	624.00	Joback Method
cpg	370.48	J/mol×K	658.08	Joback Method
cpg	382.22	J/mol×K	692.15	Joback Method
dvisc	0.0018138	Pa×s	265.19	Joback Method
dvisc	0.0010046	Pa×s	302.28	Joback Method
dvisc	0.0006331	Pa×s	339.37	Joback Method
dvisc	0.0004370	Pa×s	376.46	Joback Method
dvisc	0.0003223	Pa×s	413.54	Joback Method
dvisc	0.0002500	Pa×s	450.63	Joback Method
dvisc	0.0002015	Pa×s	487.72	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17059459&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol688.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
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