1,3-Dimethyl-2-n-Propylbenzene

Other names: 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]: 148.25

Physical Properties

Property code	Value	Unit	Source
af	0.4169		Cheméo Relay (1.0)
gf	134.89	kJ/mol	Joback Method
hf	-39.95	kJ/mol	Cheméo Relay (1.0)
hfus	17.51	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-3.98		Cheméo Relay (1.0)
logp	3.256		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1152.20		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1451.60		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1451.60		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1410.00		NIST Webbook

ripol	1410.10		NIST Webbook
tb	477.37	K	Cheméo Relay (1.0)
tc	676.64	K	Cheméo Relay (1.0)
tf	236.72	K	Cheméo Relay (1.0)
vc	0.522	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17059459&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):

KDB: https://www.cheric.org/files/research/kdb/mol/mol688.mol

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
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