1,3-Dimethyl-4-propylbenzene

Other names:	1,3-Dimethyl-4-n-Propylbenzene
	Benzene, 1,3-dimethyl-4-propyl
Inchi:	InChI=1S/C11H16/c1-4-5-11-7-6-9(2)8-10(11)3/h6-8H,4-5H2,1-3H3
InchiKey:	HPAXKQMKDWCLGU-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCCc1ccc(C)cc1C
Mol. weight [g/mol]:	148.24
CAS:	61827-85-8

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	1144.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1143.70		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1152.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1394.40		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1394.00		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	1.43841e+01
Coeff. B	-3.96829e+03
Coeff. C	-7.34040e+01
Temperature range (K), min.	354.91
Temperature range (K), max.	510.79

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R42821&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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