BENZENE, 1,3,5-TRIMETHYL-2-PROPYL-

Other names: 1,3,5-Trimethyl-2-n-propylbenzene
1,3,5-Trimethyl-2-propylbenzene
Inchi: InChI=1S/C12H18/c1-5-6-12-10(3)7-9(2)8-11(12)4/h7-8H,5-6H2,1-4H3
InchiKey: CDDRKPHVEQMWKP-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCCc1c(C)cc(C)cc1C
Mol. weight [g/mol]: 162.28

Physical Properties

Property code	Value	Unit	Source
af	0.4690		Cheméo Relay (1.0)
gf	133.68	kJ/mol	Joback Method
hf	-65.10	kJ/mol	Cheméo Relay (1.0)
hfus	19.71	kJ/mol	Joback Method
hvap	58.39	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
logp	3.564		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
ripol	1507.40		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1507.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	495.53	K	Cheméo Relay (1.0)
tc	690.69	K	Cheméo Relay (1.0)
tf	253.12	K	Cheméo Relay (1.0)
vc	0.581	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	347.28	J/mol×K	515.58	Joback Method
cpg	363.09	J/mol×K	549.37	Joback Method
cpg	378.15	J/mol×K	583.16	Joback Method
cpg	392.49	J/mol×K	616.94	Joback Method
cpg	406.14	J/mol×K	650.73	Joback Method
cpg	419.10	J/mol×K	684.52	Joback Method
cpg	431.41	J/mol×K	718.31	Joback Method
dvisc	0.0013949	Pa×s	288.98	Joback Method
dvisc	0.0008227	Pa×s	326.75	Joback Method
dvisc	0.0005414	Pa×s	364.51	Joback Method
dvisc	0.0003853	Pa×s	402.28	Joback Method
dvisc	0.0002908	Pa×s	440.05	Joback Method
dvisc	0.0002294	Pa×s	477.81	Joback Method
dvisc	0.0001874	Pa×s	515.58	Joback Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4810042&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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