

Benzene, 1,2,3-trimethyl-4-propyl

Other names:	1,2,3-Trimethyl-4-n-Propylbenzene
Inchi:	InChI=1S/C12H18/c1-5-6-12-8-7-9(2)10(3)11(12)4/h7-8H,5-6H2,1-4H3
InchiKey:	SZAIENRDRCMPRX-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCc1ccc(C)c(C)c1C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	133.68	kJ/mol	Joback Method
hf	-88.89	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.564		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1297.00		NIST Webbook
ripol	1567.60		NIST Webbook
ripol	1567.60		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	515.58	K	Joback Method
tc	718.31	K	Joback Method
tf	288.98	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/molxK	515.58	Joback Method
cpg	363.09	J/molxK	549.37	Joback Method
cpg	378.15	J/molxK	583.16	Joback Method
cpg	392.49	J/molxK	616.94	Joback Method

cpg	406.14	J/molxK	650.73	Joback Method
cpg	419.10	J/molxK	684.52	Joback Method
cpg	431.41	J/molxK	718.31	Joback Method
dvisc	0.0013949	Paxs	288.98	Joback Method
dvisc	0.0008227	Paxs	326.75	Joback Method
dvisc	0.0005414	Paxs	364.51	Joback Method
dvisc	0.0003853	Paxs	402.28	Joback Method
dvisc	0.0002908	Paxs	440.05	Joback Method
dvisc	0.0002294	Paxs	477.81	Joback Method
dvisc	0.0001874	Paxs	515.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R53016&Units=SI

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

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