

2,4,6-Trimethylcumene

Other names:	Benzene, 1,3,5-trimethyl-2-(1-methylethyl)- 1,3,5-Trimethyl-2-isopropylbenzene
Inchi:	InChI=1S/C12H18/c1-8(2)12-10(4)6-9(3)7-11(12)5/h6-8H,1-5H3
InchiKey:	OBSKMRWGMGXHFRO-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	<chem>Cc1cc(C)c(C(C)C)c(C)c1</chem>
Mol. weight [g/mol]:	162.27
CAS:	5980-96-1

Physical Properties

Property code	Value	Unit	Source
gf	131.24	kJ/mol	Joback Method
hf	-94.17	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.735		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1244.00		NIST Webbook
ripol	1478.50		NIST Webbook
ripol	1478.00		NIST Webbook
ripol	1478.00		NIST Webbook
tb	515.14	K	Joback Method
tc	722.37	K	Joback Method
tf	273.98	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	347.52	J/molxK	515.14	Joback Method
cpg	363.75	J/molxK	549.68	Joback Method
cpg	379.20	J/molxK	584.22	Joback Method
cpg	393.88	J/molxK	618.76	Joback Method
cpg	407.83	J/molxK	653.30	Joback Method
cpg	421.05	J/molxK	687.83	Joback Method
cpg	433.58	J/molxK	722.37	Joback Method
dvisc	0.0017985	Paxs	273.98	Joback Method
dvisc	0.0009540	Paxs	314.17	Joback Method
dvisc	0.0005843	Paxs	354.37	Joback Method
dvisc	0.0003955	Paxs	394.56	Joback Method
dvisc	0.0002877	Paxs	434.75	Joback Method
dvisc	0.0002209	Paxs	474.95	Joback Method
dvisc	0.0001767	Paxs	515.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5980961&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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