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: OBSKMRWMGXHFRO-UHFFFAOYSA-N
Formula: C12H18
SMILES: Cc1cc(C)c(C(C)C)c(C)c1
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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	347.52	J/mol×K	515.14	Joback Method
cpg	363.75	J/mol×K	549.68	Joback Method
cpg	379.20	J/mol×K	584.22	Joback Method
cpg	393.88	J/mol×K	618.76	Joback Method
cpg	407.83	J/mol×K	653.30	Joback Method
cpg	421.05	J/mol×K	687.83	Joback Method
cpg	433.58	J/mol×K	722.37	Joback Method
dvisc	0.0017985	Pa×s	273.98	Joback Method
dvisc	0.0009540	Pa×s	314.17	Joback Method
dvisc	0.0005843	Pa×s	354.37	Joback Method
dvisc	0.0003955	Pa×s	394.56	Joback Method
dvisc	0.0002877	Pa×s	434.75	Joback Method
dvisc	0.0002209	Pa×s	474.95	Joback Method
dvisc	0.0001767	Pa×s	515.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5980961&Units=SI
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

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