

Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-

Other names:	1,2,4-Trimethyl-5-isopropylbenzene 1-Isopropyl-2,4,5-trimethylbenzene 2,4,5-Trimethylcumene 5-Isopropyl-1,2,4-trimethylbenzene 5-Isopropylpseudocumene Benzene, 1,2,4-trimethyl-5-isopropyl Cumene, 2,4,5-trimethyl-
Inchi:	InChI=1S/C12H18/c1-8(2)12-7-10(4)9(3)6-11(12)5/h6-8H,1-5H3
InchiKey:	POOXAYBPGIHSME-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	<chem>Cc1cc(C)c(C(C)C)cc1C</chem>
Mol. weight [g/mol]:	162.27
CAS:	10222-95-4

Physical Properties

Property code	Value	Unit	Source
gf	131.24	kJ/mol	Joback Method
hf	-103.30	kJ/mol	NIST Webbook
hfus	16.19	kJ/mol	Joback Method
hvap	64.85	kJ/mol	NIST Webbook
hvap	64.90	kJ/mol	NIST Webbook
log10ws	-4.08		Crippen Method
logp	3.735		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
ripol	1234.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1476.60		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1477.00		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/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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47649e+01
Coeff. B	-4.21719e+03
Coeff. C	-7.85240e+01
Temperature range (K), min.	369.82
Temperature range (K), max.	524.62

Sources

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=C10222954&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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