

Benzene, 1-ethyl-2,3,4,5-tetramethyl

Inchi:	InChI=1S/C12H18/c1-6-12-7-8(2)9(3)10(4)11(12)5/h7H,6H2,1-5H3
InchiKey:	UCVPNSFREXDFFW-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCc1cc(C)c(C)c(C)c1C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	124.05	kJ/mol	Joback Method
hf	-100.36	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	47.23	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.483		Crippen Method
mvol	156.180	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1344.00		NIST Webbook
tb	520.56	K	Joback Method
tc	724.42	K	Joback Method
tf	301.50	K	Joback Method
vc	0.600	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.65	J/molxK	520.56	Joback Method
cpg	418.30	J/molxK	690.44	Joback Method
cpg	405.49	J/molxK	656.47	Joback Method
cpg	392.03	J/molxK	622.49	Joback Method
cpg	377.91	J/molxK	588.51	Joback Method
cpg	363.12	J/molxK	554.54	Joback Method
cpg	430.49	J/molxK	724.42	Joback Method
dvisc	0.0001820	Paxs	520.56	Joback Method

dvisc	0.0002187	Paxs	484.05	Joback Method
dvisc	0.0002709	Paxs	447.54	Joback Method
dvisc	0.0003485	Paxs	411.03	Joback Method
dvisc	0.0004708	Paxs	374.52	Joback Method
dvisc	0.0006788	Paxs	338.01	Joback Method
dvisc	0.0010695	Paxs	301.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R52961&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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