

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

Inchi:	InChI=1S/C12H16/c1-8(2)12-7-10(4)9(3)6-11(12)5/h6-7H,1H2,2-5H3
InchiKey:	IFKGNSBJIQOCSH-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	<chem>C=C(C)c1cc(C)c(C)cc1C</chem>
Mol. weight [g/mol]:	160.26
CAS:	54340-84-0

Physical Properties

Property code	Value	Unit	Source
gf	212.97	kJ/mol	Joback Method
hf	26.75	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.645		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	512.14	K	Joback Method
tc	723.12	K	Joback Method
tf	273.26	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.63	J/molxK	512.14	Joback Method
cpg	344.06	J/molxK	547.30	Joback Method
cpg	358.70	J/molxK	582.47	Joback Method
cpg	372.59	J/molxK	617.63	Joback Method
cpg	385.75	J/molxK	652.79	Joback Method
cpg	398.20	J/molxK	687.96	Joback Method
cpg	409.97	J/molxK	723.12	Joback Method

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=C54340840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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