

Benzene, 1,2,3,5-tetramethyl-4-(1-methylethyl)

Inchi:	InChI=1S/C13H20/c1-8(2)13-10(4)7-9(3)11(5)12(13)6/h7-8H,1-6H3
InchiKey:	GNMPAJFUVPIAQD-UHFFFAOYSA-N
Formula:	C13H20
SMILES:	Cc1cc(C)c(C(C)C)c(C)c1C
Mol. weight [g/mol]:	176.30

Physical Properties

Property code	Value	Unit	Source
gf	130.03	kJ/mol	Joback Method
hf	-126.28	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.044		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	1374.00		NIST Webbook
tb	543.00	K	Joback Method
tc	748.22	K	Joback Method
tf	297.77	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.00	J/molxK	543.00	Joback Method
cpg	471.08	J/molxK	714.02	Joback Method
cpg	457.34	J/molxK	679.81	Joback Method
cpg	442.88	J/molxK	645.61	Joback Method
cpg	427.68	J/molxK	611.41	Joback Method
cpg	411.72	J/molxK	577.20	Joback Method
cpg	484.11	J/molxK	748.22	Joback Method
dvisc	0.0001634	Paxs	543.00	Joback Method
dvisc	0.0002016	Paxs	502.13	Joback Method

dvisc	0.0002581	Paxs	461.26	Joback Method
dvisc	0.0003468	Paxs	420.38	Joback Method
dvisc	0.0004965	Paxs	379.51	Joback Method
dvisc	0.0007751	Paxs	338.64	Joback Method
dvisc	0.0013675	Paxs	297.77	Joback Method

Sources

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=R550051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:

<https://www.chemeo.com/cid/22-057-4/Benzene-1-2-3-5-tetramethyl-4-1-methylethyl.pdf>

Generated by Cheméo on 2024-04-19 02:08:12.419364212 +0000 UTC m=+15781741.339941528.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.