

1,4-Hexadiene, 2,3,4,5-tetramethyl-

Other names:	2,3,4,5-Tetramethylhexa-1,4-diene 2,3,4,5-Tetramethyl-1,4-hexadiene
Inchi:	InChI=1S/C10H18/c1-7(2)9(5)10(6)8(3)4/h9H,1H2,2-6H3
InchiKey:	ZPYYCZZBNXDIMQ-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C=C(C)C(C)C(C)=C(C)C
Mol. weight [g/mol]:	138.25
CAS:	51504-54-2

Physical Properties

Property code	Value	Unit	Source
gf	173.29	kJ/mol	Joback Method
hf	-41.73	kJ/mol	Joback Method
hfus	13.12	kJ/mol	Joback Method
hvap	36.99	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	428.24	K	Joback Method
tc	616.29	K	Joback Method
tf	138.74	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.89	J/mol×K	428.24	Joback Method
cpg	299.52	J/mol×K	459.58	Joback Method
cpg	314.39	J/mol×K	490.92	Joback Method
cpg	328.52	J/mol×K	522.27	Joback Method
cpg	341.94	J/mol×K	553.61	Joback Method
cpg	354.70	J/mol×K	584.95	Joback Method
cpg	366.81	J/mol×K	616.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51504542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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