

1,1,3,5-Tetramethylcyclohexane

Inchi:	InChI=1S/C10H20/c1-8-5-9(2)7-10(3,4)6-8/h8-9H,5-7H2,1-4H3
InchiKey:	WOJSMJIXPQLESQ-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CC1CC(C)CC(C)(C)C1
Mol. weight [g/mol]:	140.27

Physical Properties

Property code	Value	Unit	Source
gf	36.86	kJ/mol	Joback Method
hf	-220.85	kJ/mol	Joback Method
hfus	9.33	kJ/mol	Joback Method
hvap	36.51	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.469		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	890.00		NIST Webbook
rinpol	898.70		NIST Webbook
rinpol	898.70		NIST Webbook
tb	438.65	K	Joback Method
tc	643.42	K	Joback Method
tf	225.26	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.31	J/mol×K	438.65	Joback Method
cpg	321.00	J/mol×K	472.78	Joback Method
cpg	340.50	J/mol×K	506.91	Joback Method
cpg	358.88	J/mol×K	541.03	Joback Method
cpg	376.24	J/mol×K	575.16	Joback Method
cpg	392.65	J/mol×K	609.29	Joback Method
cpg	408.21	J/mol×K	643.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R141112&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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