

1,4,4,7-tetramethylcycloheptene

Inchi:

InChI=1S/C11H20/c1-9-5-7-11(3,4)8-6-10(9)2/h5,10H,6-8H2,1-4H3

InchiKey:

SICYNZBBKVUCOS-UHFFFAOYSA-N

Formula:

C11H20

SMILES:

CC1=CCC(C)(C)CCC1C

Mol. weight [g/mol]:

152.28

Physical Properties

Property code	Value	Unit	Source
gf	61.22	kJ/mol	Joback Method
hf	-181.00	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	40.18	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.779		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1029.50		NIST Webbook
tb	474.61	K	Joback Method
tc	688.62	K	Joback Method
tf	250.53	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.04	J/mol×K	474.61	Joback Method
cpg	353.50	J/mol×K	510.28	Joback Method
cpg	372.75	J/mol×K	545.95	Joback Method
cpg	390.90	J/mol×K	581.62	Joback Method
cpg	408.02	J/mol×K	617.29	Joback Method
cpg	424.23	J/mol×K	652.96	Joback Method
cpg	439.62	J/mol×K	688.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492054&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
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/42-675-6/1-4-4-7-tetramethylcycloheptene.pdf>

Generated by Cheméo on 2025-12-06 04:23:28.069190749 +0000 UTC m=+4743205.599231403.

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