

2-HEPTENE, 2,6-DIMETHYL-

Other names:	2,6-Dimethyl-2-heptene
Inchi:	InChI=1S/C9H18/c1-8(2)6-5-7-9(3)4/h6,9H,5,7H2,1-4H3
InchiKey:	JDJYGSMZGYTCML-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC(C)=CCCC(C)C
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
hf	-142.30	kJ/mol	Cheméo Relay (1.0)
hfus	14.43	kJ/mol	Joback Method
hvap	40.83	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	409.00 ± 3.00	K	NIST Webbook
tc	574.05	K	Cheméo Relay (1.0)
tf	167.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.98	J/mol×K	408.92	Joback Method
cpg	272.62	J/mol×K	438.66	Joback Method
cpg	286.61	J/mol×K	468.40	Joback Method
cpg	299.98	J/mol×K	498.14	Joback Method
cpg	312.75	J/mol×K	527.89	Joback Method
cpg	324.94	J/mol×K	557.63	Joback Method
cpg	336.58	J/mol×K	587.37	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C5557982&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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