

4,6-dimethyl-3-heptene

Inchi:	InChI=1S/C9H18/c1-5-6-9(4)7-8(2)3/h6,8H,5,7H2,1-4H3/b9-6+
InchiKey:	FALJCIDAIJRLIF-RMKNXTFCSA-N
Formula:	C9H18
SMILES:	CCC=C(C)CC(C)C
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	94.13	kJ/mol	Joback Method
hf	-126.94	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	35.28	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mvol	133.370	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
tb	408.92	K	Joback Method
tc	587.37	K	Joback Method
tf	157.15	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R141414&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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