

3,5-Dimethyl-3-heptene

Inchi:	InChI=1S/C9H18/c1-5-8(3)7-9(4)6-2/h7-8H,5-6H2,1-4H3/b9-7+
InchiKey:	OXOLZWHOQAEIAW-VQHVLOKHSA-N
Formula:	C9H18
SMILES:	CCC(C)=CC(C)CC
Mol. weight [g/mol]:	126.24
CAS:	59643-68-4

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
mcvol	133.370	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	836.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	833.00		NIST Webbook
tb	408.92	K	Joback Method
tc	587.37	K	Joback Method
tf	157.15	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59643684&Units=SI
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

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

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