

3,4-Octadiene, 7-methyl-

Inchi:	InChI=1S/C9H16/c1-4-5-6-7-8-9(2)3/h5,7,9H,4,8H2,1-3H3
InchiKey:	GOFRIZQMGVLGIN-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CCC=C=CCC(C)C
Mol. weight [g/mol]:	124.22
CAS:	37050-05-8

Physical Properties

Property code	Value	Unit	Source
gf	230.96	kJ/mol	Joback Method
hf	45.63	kJ/mol	Joback Method
hfus	17.88	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.154		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	412.31	K	Joback Method
tc	598.48	K	Joback Method
tf	177.62	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.91	J/mol×K	412.31	Joback Method
cpg	261.51	J/mol×K	443.34	Joback Method
cpg	274.56	J/mol×K	474.37	Joback Method
cpg	287.05	J/mol×K	505.40	Joback Method
cpg	299.02	J/mol×K	536.42	Joback Method
cpg	310.48	J/mol×K	567.45	Joback Method
cpg	321.43	J/mol×K	598.48	Joback Method

Sources

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=C37050058&Units=SI
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
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
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/23-653-1/3-4-Octadiene-7-methyl.pdf>

Generated by Cheméo on 2025-12-21 21:26:47.491126129 +0000 UTC m=+6100605.021166799.

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