

(E)-4,8-Dimethyl-1,3,9-nonatriene

Inchi:	InChI=1S/C11H18/c1-5-7-11(4)9-6-8-10(2)3/h5,7H,1-2,6,8-9H2,3-4H3/b11-7+
InchiKey:	ZJBYNALFMUYJOB-YRNVUSSQSA-N
Formula:	C11H18
SMILES:	C=CC=C(C)CCCC(=C)C
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	280.54	kJ/mol	Joback Method
hf	78.13	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.865		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1105.00		NIST Webbook
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tb	448.36	K	Joback Method
tc	630.91	K	Joback Method
tf	177.21	K	Joback Method
vc	0.596	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.58	J/mol×K	448.36	Joback Method
cpg	325.91	J/mol×K	478.78	Joback Method
cpg	340.48	J/mol×K	509.21	Joback Method
cpg	354.32	J/mol×K	539.63	Joback Method
cpg	367.46	J/mol×K	570.06	Joback Method
cpg	379.94	J/mol×K	600.48	Joback Method
cpg	391.79	J/mol×K	630.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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