

(E)-4,8-Dimethyl-1,3,7-nonatriene

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

Physical Properties

Property code	Value	Unit	Source
gf	272.92	kJ/mol	Joback Method
hf	69.92	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.865		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
ripol	1097.00		NIST Webbook
ripol	1106.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1084.00		NIST Webbook
ripol	1113.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1118.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1314.00		NIST Webbook
ripol	1303.00		NIST Webbook
ripol	1302.00		NIST Webbook
ripol	1306.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1309.00		NIST Webbook
ripol	1309.00		NIST Webbook
tb	455.84	K	Joback Method

tc	643.33	K	Joback Method
tf	173.89	K	Joback Method
vc	0.595	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.66	J/mol×K	455.84	Joback Method
cpg	327.28	J/mol×K	487.09	Joback Method
cpg	342.08	J/mol×K	518.34	Joback Method
cpg	356.08	J/mol×K	549.58	Joback Method
cpg	369.34	J/mol×K	580.83	Joback Method
cpg	381.90	J/mol×K	612.08	Joback Method
cpg	393.80	J/mol×K	643.33	Joback Method

Sources

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=R292116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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