4,8-Dimethyl-1,3,7-nonatriene

Other names:	1,3,7-Nonatriene, 4,8-dimethyl- 4,8-Dimethyl-1,3,7-nonatriene (Isomer 1) 4,8-Dimethylnona-1,3,7-triene (Isomer 2) 4,8 Dimethylnona-1,3,7-triene
Inchi:	InChI=1S/C11H18/c1-5-7-11(4)9-6-8-10(2)3/h5,7-8H,1,6,9H2,2-4H3
InchiKey:	LUKZREJJLWEWQM-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C=CC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	150.26
CAS:	51911-82-1

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
rinpol	1116.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1114.10		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1114.10		NIST Webbook
rinpol	1103.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1301.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
tb	455.84	K	Joback Method
tc	643.33	K	Joback Method
tf	173.89	K	Joback Method

vc	0.595	m3/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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51911821&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume