

1,8-Nonadiene, 2,4,6,8-tetramethyl, # 2

Inchi:	InChI=1S/C13H24/c1-10(2)7-12(5)9-13(6)8-11(3)4/h12-13H,1,3,7-9H2,2,4-6H3
InchiKey:	ZWOKFAVFJDZGAW-UHFFFAOYSA-N
Formula:	C13H24
SMILES:	C=C(C)CC(C)CC(C)CC(=C)C
Mol. weight [g/mol]:	180.33

Physical Properties

Property code	Value	Unit	Source
gf	212.28	kJ/mol	Joback Method
hf	-90.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.581		Crippen Method
mvol	185.430	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	489.08	K	Joback Method
tc	667.82	K	Joback Method
tf	174.83	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.47	J/mol×K	489.08	Joback Method
cpg	436.41	J/mol×K	518.87	Joback Method
cpg	453.54	J/mol×K	548.66	Joback Method
cpg	469.88	J/mol×K	578.45	Joback Method
cpg	485.47	J/mol×K	608.24	Joback Method
cpg	500.33	J/mol×K	638.03	Joback Method
cpg	514.49	J/mol×K	667.82	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=R568126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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