3,7-NONADIEN-2-ONE, 4,8-DIMETHYL-

Other names: 4,8-Dimethyl-3,7-nonadien-2-one
4,8-Dimethylnona-3,7-dien-2-one
Inchi: InChI=1S/C11H18O/c1-9(2)6-5-7-10(3)8-11(4)12/h6,8H,5,7H2,1-4H3/b10-8+
InchiKey: QAFYGHBGWCPRCI-NTMALXAHSA-N
Formula: C11H18O
SMILES: CC(=O)/C=C(/C)CCC=C(C)C
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
hf	-221.50	kJ/mol	Cheméo Relay (1.0)
hfus	23.63	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-2.81		Cheméo Relay (1.0)
logp	3.268		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1240.80		NIST Webbook
rinpol	1240.80		NIST Webbook
tb	498.73	K	Cheméo Relay (1.0)
tc	678.80	K	Cheméo Relay (1.0)
tf	221.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.26	J/mol×K	513.03	Joback Method
cpg	368.28	J/mol×K	545.28	Joback Method
cpg	382.49	J/mol×K	577.52	Joback Method
cpg	395.95	J/mol×K	609.77	Joback Method
cpg	408.69	J/mol×K	642.02	Joback Method
cpg	420.75	J/mol×K	674.26	Joback Method
cpg	432.17	J/mol×K	706.51	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C817889&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point