

6,8-Nonadien-2-one, 6-methyl-5-(1-methylethylidene)-

Inchi:	InChI=1S/C13H20O/c1-6-7-11(4)13(10(2)3)9-8-12(5)14/h6-7H,1,8-9H2,2-5H3/b11-7+
InchiKey:	KUZCXMAGIONJAL-YRNVUSSQSA-N
Formula:	C13H20O
SMILES:	C=CC=C(C)C(CCC(C)=O)=C(C)C
Mol. weight [g/mol]:	192.30
CAS:	60714-16-1

Physical Properties

Property code	Value	Unit	Source
gf	152.29	kJ/mol	Joback Method
hf	-93.73	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	50.76	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1767.00		NIST Webbook
tb	555.35	K	Joback Method
tc	751.01	K	Joback Method
tf	232.40	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.69	J/molxK	555.35	Joback Method
cpg	444.74	J/molxK	587.96	Joback Method
cpg	459.90	J/molxK	620.57	Joback Method
cpg	474.23	J/molxK	653.18	Joback Method
cpg	487.77	J/molxK	685.79	Joback Method

cpg	500.58	J/mol×K	718.40	Joback Method
cpg	512.71	J/mol×K	751.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60714161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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