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=C/C=C(\C)C(CCC(C)=O)=C(C)C

Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
hfus	26.22	kJ/mol	Joback Method
ie	7.84	eV	Cheméo Relay (1.0)
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1767.00		NIST Webbook
tb	524.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60714161&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature