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

Other names: (.+/-.)-Solanone
(6E)-5-Isopropyl-8-methyl-6,8-nonadien-2-one
(E)-5-Isopropyl-8-methylnona-6,8-dien-2-one
Solanone
(E)-Solanone

Inchi: InChI=1S/C13H22O/c1-10(2)6-8-13(11(3)4)9-7-12(5)14/h6,8,11,13H,1,7,9H2,2-5H3/b8-6

InchiKey: PQDRXUSSKFWCFA-SOFGYWHQSA-N

Formula: C13H22O

SMILES: C=C(C)C=CC(CCC(C)=O)C(C)C

Mol. weight [g/mol]: 194.31

CAS: 54868-48-3

Physical Properties

Property code	Value	Unit	Source
gf	84.29	kJ/mol	Joback Method
hf	-201.93	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	49.87	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.760		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
ripol	1756.00		NIST Webbook
ripol	1756.00		NIST Webbook
tb	550.55	K	Joback Method
tc	739.38	K	Joback Method
tf	235.40	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.23	J/mol×K	550.55	Joback Method
cpg	464.96	J/mol×K	582.02	Joback Method

cpg	480.83	J/mol×K	613.49	Joback Method
cpg	495.89	J/mol×K	644.97	Joback Method
cpg	510.17	J/mol×K	676.44	Joback Method
cpg	523.72	J/mol×K	707.91	Joback Method
cpg	536.55	J/mol×K	739.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54868483&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume