(Z) -3-hydroxy-5,9-dimethyldeca-4,8-dien-2-on (R,S)

Inchi: InChI=1S/C12H20O2/c1-9(2)6-5-7-10(3)8-12(14)11(4)13/h6,8,12,14H,5,7H2,1-4H3/b10-8

InchiKey: DPGJGJBHBQMSDM-CUZBXDDWSA-N

Formula: C12H20O2

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

Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-74.68	kJ/mol	Joback Method
hf	-346.24	kJ/mol	Joback Method
hfus	26.78	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.629		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
ripol	1692.00		NIST Webbook
tb	627.65	K	Joback Method
tc	812.54	K	Joback Method
tf	282.67	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.04	J/mol×K	627.65	Joback Method
cpg	474.35	J/mol×K	658.47	Joback Method
cpg	486.96	J/mol×K	689.28	Joback Method
cpg	498.93	J/mol×K	720.10	Joback Method
cpg	510.30	J/mol×K	750.91	Joback Method
cpg	521.10	J/mol×K	781.73	Joback Method
cpg	531.38	J/mol×K	812.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522695&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
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