2-hydroxy-5,9-dimethyl-dec-8-en-3-on (R, S)

Inchi: InChI=1S/C12H22O2/c1-9(2)6-5-7-10(3)8-12(14)11(4)13/h6,10-11,13H,5,7-8H2,1-4H3/t1
InchiKey: NXGKHHATOTXWAM-MNOVXSKESA-N
Formula: C12H22O2
SMILES: CC(C)=CCCC(C)CC(=O)C(C)O
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-148.79	kJ/mol	Joback Method
hf	-458.95	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.709		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1432.00		NIST Webbook
ripol	1979.00		NIST Webbook
tb	623.17	K	Joback Method
tc	802.18	K	Joback Method
tf	286.71	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.68	J/mol×K	623.17	Joback Method
cpg	496.60	J/mol×K	653.00	Joback Method
cpg	509.84	J/mol×K	682.84	Joback Method
cpg	522.44	J/mol×K	712.67	Joback Method
cpg	534.41	J/mol×K	742.51	Joback Method
cpg	545.80	J/mol×K	772.34	Joback Method
cpg	556.63	J/mol×K	802.18	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522660&Units=SI
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
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