1,3-Cyclohexadien-2-ol, 3-methyl-5-(1,5-dimethyl-3-oxo-4-hexen-1-yl)

Inchi: InChI=1S/C15H22O2/c1-10(2)7-14(16)9-11(3)13-5-6-15(17)12(4)8-13/h6-8,11,13,17H,5,

InchiKey: DDHVYJOVPXXZJQ-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: CC(C)=CC(=O)CC(C)C1C=C(C)C(O)=CC1

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-55.98	kJ/mol	Joback Method
hf	-368.65	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	74.40	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.956		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	720.08	K	Joback Method
tc	920.97	K	Joback Method
tf	369.46	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.93	J/mol×K	720.08	Joback Method
cpg	600.08	J/mol×K	753.56	Joback Method
cpg	614.34	J/mol×K	787.04	Joback Method
cpg	627.75	J/mol×K	820.52	Joback Method
cpg	640.36	J/mol×K	854.00	Joback Method
cpg	652.21	J/mol×K	887.49	Joback Method
cpg	663.33	J/mol×K	920.97	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=R400085&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume