4-(1,5-Dimethylhex-4-enyl)cyclohex-2-enone

Other names: 4-(6-Methylhept-5-en-2-yl)cyclohex-2-enone
Inchi: InChI=1S/C14H22O/c1-11(2)5-4-6-12(3)13-7-9-14(15)10-8-13/h5,7,9,12-13H,4,6,8,10H2
InchiKey: CIIUTVUZULBJKL-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC(C)=CCCC(C)C1C=CC(=O)CC1
Mol. weight [g/mol]: 206.32
CAS: 1723-80-4

Physical Properties

Property code	Value	Unit	Source
gf	68.05	kJ/mol	Joback Method
hf	-255.74	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1697.80		NIST Webbook
rinpol	1697.80		NIST Webbook
tb	609.85	K	Joback Method
tc	828.69	K	Joback Method
tf	289.86	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.61	J/mol×K	609.85	Joback Method
cpg	522.16	J/mol×K	646.32	Joback Method
cpg	541.51	J/mol×K	682.80	Joback Method
cpg	559.71	J/mol×K	719.27	Joback Method
cpg	576.77	J/mol×K	755.74	Joback Method
cpg	592.74	J/mol×K	792.21	Joback Method

cpg	607.63	J/mol×K	828.69	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=C1723804&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