6,10-Dimethyl-4,5,9-undecatrien-2-one

Inchi: InChI=1S/C13H20O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6-7H,5,8,10H2,1-4H3
InchiKey: KLTSFSBBACTSHL-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(=O)CC=C=C(C)CCC=C(C)C
Mol. weight [g/mol]: 192.30
CAS: 16647-05-5

Physical Properties

Property code	Value	Unit	Source
chs	-7781.60 ± 2.50	kJ/mol	NIST Webbook
gf	201.28	kJ/mol	Joback Method
hf	-46.59	kJ/mol	Joback Method
hfs	-192.10 ± 2.50	kJ/mol	NIST Webbook
hfus	30.94	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.813		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
tb	562.06	K	Joback Method
tc	760.95	K	Joback Method
tf	254.63	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.40	J/mol×K	727.80	Joback Method
cpg	432.27	J/mol×K	562.06	Joback Method
cpg	448.28	J/mol×K	595.21	Joback Method
cpg	463.46	J/mol×K	628.36	Joback Method
cpg	477.85	J/mol×K	661.50	Joback Method
cpg	491.48	J/mol×K	694.65	Joback Method
cpg	516.64	J/mol×K	760.95	Joback Method

cpl	413.40	J/mol×K	313.65	NIST Webbook
hvapt	63.60 ± 1.40	kJ/mol	385.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16647055&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume