3,5,9-Undecatrien-2-one, 6,10-dimethyl, #2

Inchi: InChI=1S/C13H20O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6-7,9-10H,5,8H2,1-4H3/b10-6+
InchiKey: JXJIQCXXJGRKRJ-KOOBJXAQSA-N
Formula: C13H20O
SMILES: CC(=O)C=CC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	153.22	kJ/mol	Joback Method
hf	-92.15	kJ/mol	Joback Method
hfus	29.01	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	562.95	K	Joback Method
tc	759.70	K	Joback Method
tf	243.04	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.05	J/mol×K	562.95	Joback Method
cpg	445.99	J/mol×K	595.74	Joback Method
cpg	461.03	J/mol×K	628.53	Joback Method
cpg	475.23	J/mol×K	661.33	Joback Method
cpg	488.64	J/mol×K	694.12	Joback Method
cpg	501.32	J/mol×K	726.91	Joback Method
cpg	513.34	J/mol×K	759.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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