3-Methyl-2-pent-2-enyl-cyclopent-2-enone

Other names: 3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one
Inchi: InChI=1S/C11H16O/c1-3-4-5-6-10-9(2)7-8-11(10)12/h4-5H,3,6-8H2,1-2H3/b5-4+
InchiKey: XMLSXPIVAXONDL-SNAWJCMRSA-N
Formula: C11H16O
SMILES: CCC=CCC1=C(C)CCC1=O
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	54.33	kJ/mol	Joback Method
hf	-175.19	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.47	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.022		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	552.13	K	Joback Method
tc	768.56	K	Joback Method
tf	317.81	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.55	J/mol×K	552.13	Joback Method
cpg	364.59	J/mol×K	588.20	Joback Method
cpg	379.80	J/mol×K	624.27	Joback Method
cpg	394.21	J/mol×K	660.34	Joback Method
cpg	407.84	J/mol×K	696.41	Joback Method
cpg	420.71	J/mol×K	732.49	Joback Method
cpg	432.85	J/mol×K	768.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U193436&Units=SI

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