2-Methyl-6-methylene-7-octen-3-one

Inchi: InChI=1S/C10H16O/c1-5-9(4)6-7-10(11)8(2)3/h5,8H,1,4,6-7H2,2-3H3
InchiKey: IYFQOCPXUHQIMN-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=CC(=C)CCC(=O)C(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	69.09	kJ/mol	Joback Method
hf	-126.52	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	42.95	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1098.00		NIST Webbook
tb	474.87	K	Joback Method
tc	661.71	K	Joback Method
tf	219.91	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.00	J/mol×K	474.87	Joback Method
cpg	320.91	J/mol×K	506.01	Joback Method
cpg	334.15	J/mol×K	537.15	Joback Method
cpg	346.73	J/mol×K	568.29	Joback Method
cpg	358.69	J/mol×K	599.43	Joback Method
cpg	370.05	J/mol×K	630.57	Joback Method
cpg	380.83	J/mol×K	661.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R589445&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

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

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