6-Octen-2-one, 7-methyl-3-methylene-

Inchi: InChI=1S/C10H16O/c1-8(2)6-5-7-9(3)10(4)11/h6H,3,5,7H2,1-2,4H3
InchiKey: SONVLKMIYCZSIS-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C(CCC=C(C)C)C(C)=O
Mol. weight [g/mol]: 152.23
CAS: 42809-05-2

Physical Properties

Property code	Value	Unit	Source
gf	55.36	kJ/mol	Joback Method
hf	-139.24	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
tb	482.67	K	Joback Method
tc	673.70	K	Joback Method
tf	217.63	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.42	J/mol×K	482.67	Joback Method
cpg	321.41	J/mol×K	514.51	Joback Method
cpg	334.68	J/mol×K	546.35	Joback Method
cpg	347.26	J/mol×K	578.19	Joback Method
cpg	359.18	J/mol×K	610.02	Joback Method
cpg	370.49	J/mol×K	641.86	Joback Method
cpg	381.20	J/mol×K	673.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42809052&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume