2-Octen-6-one, 2,5-dimethyl

Inchi: InChI=1S/C10H18O/c1-5-10(11)9(4)7-6-8(2)3/h6,9H,5,7H2,1-4H3
InchiKey: WKQWDIFHKYWRTA-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CCC(=O)C(C)CC=C(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-26.37	kJ/mol	Joback Method
hf	-260.16	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.958		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1110.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1381.00		NIST Webbook
tb	485.67	K	Joback Method
tc	673.48	K	Joback Method
tf	218.35	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.34	J/mol×K	485.67	Joback Method
cpg	340.07	J/mol×K	516.97	Joback Method
cpg	354.09	J/mol×K	548.27	Joback Method
cpg	367.43	J/mol×K	579.57	Joback Method
cpg	380.11	J/mol×K	610.87	Joback Method
cpg	392.16	J/mol×K	642.17	Joback Method
cpg	403.61	J/mol×K	673.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R126019&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume