7-Octen-4-one, 3,6-dimethyl

Inchi: InChI=1S/C10H18O/c1-5-8(3)7-10(11)9(4)6-2/h5,8-9H,1,6-7H2,2-4H3
InchiKey: JWWIOZVCPKZXRH-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=CC(C)CC(=O)C(C)CC
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-12.64	kJ/mol	Joback Method
hf	-247.44	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	43.15	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1125.00		NIST Webbook
ripol	1545.00		NIST Webbook
tb	477.87	K	Joback Method
tc	661.58	K	Joback Method
tf	220.63	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.68	J/mol×K	477.87	Joback Method
cpg	391.42	J/mol×K	630.97	Joback Method
cpg	379.32	J/mol×K	600.35	Joback Method
cpg	366.62	J/mol×K	569.73	Joback Method
cpg	353.29	J/mol×K	539.11	Joback Method
cpg	339.32	J/mol×K	508.49	Joback Method
cpg	402.93	J/mol×K	661.58	Joback Method
dvisc	0.0002440	Pa×s	477.87	Joback Method

dvisc	0.0003331	Pa×s	435.00	Joback Method
dvisc	0.0004867	Pa×s	392.12	Joback Method
dvisc	0.0007805	Pa×s	349.25	Joback Method
dvisc	0.0014286	Pa×s	306.38	Joback Method
dvisc	0.0031833	Pa×s	263.50	Joback Method
dvisc	0.0096846	Pa×s	220.63	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=R409344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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