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

Other names: 6-methyl-7-octen-2-one
Inchi: InChI=1S/C9H16O/c1-4-8(2)6-5-7-9(3)10/h4,8H,1,5-7H2,2-3H3
InchiKey: AQWAXHULODKDEJ-UHFFFAOYSA-N
Formula: C9H16O
SMILES: C=CC(C)CCCC(C)=O
Mol. weight [g/mol]: 140.22
CAS: 35215-49-7

Physical Properties

Property code	Value	Unit	Source
gf	-18.62	kJ/mol	Joback Method
hf	-221.52	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	41.32	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
ripol	1429.00		NIST Webbook
tb	455.43	K	Joback Method
tc	636.92	K	Joback Method
tf	224.36	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.01	J/mol×K	455.43	Joback Method
cpg	341.89	J/mol×K	606.68	Joback Method
cpg	330.83	J/mol×K	576.43	Joback Method
cpg	319.22	J/mol×K	546.18	Joback Method
cpg	307.06	J/mol×K	515.93	Joback Method
cpg	294.33	J/mol×K	485.68	Joback Method
cpg	352.44	J/mol×K	636.92	Joback Method

dvisc	0.0002706	Pa×s	455.43	Joback Method
dvisc	0.0003578	Pa×s	416.92	Joback Method
dvisc	0.0005007	Pa×s	378.41	Joback Method
dvisc	0.0007561	Pa×s	339.89	Joback Method
dvisc	0.0012688	Pa×s	301.38	Joback Method
dvisc	0.0024776	Pa×s	262.87	Joback Method
dvisc	0.0060877	Pa×s	224.36	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=C35215497&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume