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

Other names: 7-Methyl-3-octen-2-one
7-methyloct-3-en-2-one
Inchi: InChI=1S/C9H16O/c1-8(2)6-4-5-7-9(3)10/h5,7-8H,4,6H2,1-3H3/b7-5+
InchiKey: QFSMRIFNMXHJQK-FNORWQNLSA-N
Formula: C9H16O
SMILES: CC(=O)C=CCCC(C)C
Mol. weight [g/mol]: 140.22
CAS: 33046-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-26.24	kJ/mol	Joback Method
hf	-229.73	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	41.94	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.568		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1062.00		NIST Webbook
ripol	1317.00		NIST Webbook
tb	462.91	K	Joback Method
tc	649.25	K	Joback Method
tf	221.04	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.62	J/mol×K	462.91	Joback Method
cpg	295.21	J/mol×K	493.97	Joback Method
cpg	308.15	J/mol×K	525.02	Joback Method
cpg	320.47	J/mol×K	556.08	Joback Method
cpg	332.19	J/mol×K	587.14	Joback Method

cpg	343.33	J/mol×K	618.19	Joback Method
cpg	353.92	J/mol×K	649.25	Joback Method
dvisc	0.0064413	Pa×s	221.04	Joback Method
dvisc	0.0023944	Pa×s	261.35	Joback Method
dvisc	0.0011596	Pa×s	301.66	Joback Method
dvisc	0.0006662	Pa×s	341.97	Joback Method
dvisc	0.0004302	Pa×s	382.29	Joback Method
dvisc	0.0003020	Pa×s	422.60	Joback Method
dvisc	0.0002255	Pa×s	462.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33046810&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
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

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