5-Octen-4-one, 7-methyl-

Other names: 7-methyl-5-octen-4-one
Inchi: InChI=1S/C9H16O/c1-4-5-9(10)7-6-8(2)3/h6-8H,4-5H2,1-3H3/b7-6+
InchiKey: KBOYTXRTSGPWID-VOTSOKGWSA-N
Formula: C9H16O
SMILES: CCCC(=O)C=CC(C)C
Mol. weight [g/mol]: 140.22
CAS: 32064-78-1

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
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27643e+01
Coeff. B	-3.39561e+03
Coeff. C	-6.80630e+01
Temperature range (K), min.	340.22
Temperature range (K), max.	523.67

Sources

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=C32064781&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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