3-Decanone, 2-methyl-

Other names: 2-Methyl-3-decanone
2-methyldecan-3-one
Inchi: InChI=1S/C11H22O/c1-4-5-6-7-8-9-11(12)10(2)3/h10H,4-9H2,1-3H3
InchiKey: HJSFZKMTFMWEAQ-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCCCCCCC(=O)C(C)C
Mol. weight [g/mol]: 170.29
CAS: 5463-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-89.62	kJ/mol	Joback Method
hf	-388.23	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.572		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
tb	504.51	K	Joback Method
tc	679.38	K	Joback Method
tf	248.66	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.41	J/mol×K	504.51	Joback Method
cpg	404.02	J/mol×K	533.65	Joback Method
cpg	418.97	J/mol×K	562.80	Joback Method
cpg	433.29	J/mol×K	591.94	Joback Method
cpg	446.99	J/mol×K	621.09	Joback Method
cpg	460.10	J/mol×K	650.23	Joback Method
cpg	472.61	J/mol×K	679.38	Joback Method

dvisc	0.0065882	Pa×s	248.66	Joback Method
dvisc	0.0025234	Pa×s	291.30	Joback Method
dvisc	0.0012349	Pa×s	333.94	Joback Method
dvisc	0.0007105	Pa×s	376.59	Joback Method
dvisc	0.0004574	Pa×s	419.23	Joback Method
dvisc	0.0003195	Pa×s	461.87	Joback Method
dvisc	0.0002371	Pa×s	504.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45783e+01
Coeff. B	-4.18822e+03
Coeff. C	-7.76060e+01
Temperature range (K), min.	370.68
Temperature range (K), max.	529.57

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=C5463821&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

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