5-Undecanone, 2-methyl-

Other names: 2-Methyl-5-undecanone
Inchi: InChI=1S/C12H24O/c1-4-5-6-7-8-12(13)10-9-11(2)3/h11H,4-10H2,1-3H3
InchiKey: JLTHSCDXCKBHCZ-UHFFFAOYSA-N
Formula: C12H24O
SMILES: CCCCCCC(=O)CCC(C)C
Mol. weight [g/mol]: 184.32
CAS: 50639-02-6

Physical Properties

Property code	Value	Unit	Source
gf	-81.20	kJ/mol	Joback Method
hf	-408.87	kJ/mol	Joback Method
hfus	24.91	kJ/mol	Joback Method
hvap	48.66	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.962		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
tb	527.39	K	Joback Method
tc	700.81	K	Joback Method
tf	259.93	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.53	J/mol×K	527.39	Joback Method
cpg	511.43	J/mol×K	671.91	Joback Method
cpg	497.75	J/mol×K	643.00	Joback Method
cpg	483.44	J/mol×K	614.10	Joback Method
cpg	468.47	J/mol×K	585.20	Joback Method
cpg	452.84	J/mol×K	556.29	Joback Method
cpg	524.50	J/mol×K	700.81	Joback Method
dvisc	0.0002185	Pa×s	527.39	Joback Method

dvisc	0.0002955	Pa×s	482.81	Joback Method
dvisc	0.0004250	Pa×s	438.24	Joback Method
dvisc	0.0006635	Pa×s	393.66	Joback Method
dvisc	0.0011609	Pa×s	349.08	Joback Method
dvisc	0.0023924	Pa×s	304.51	Joback Method
dvisc	0.0063181	Pa×s	259.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45662e+01
Coeff. B	-4.31660e+03
Coeff. C	-8.25270e+01
Temperature range (K), min.	384.84
Temperature range (K), max.	548.95

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50639026&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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