

3-Decanone

Other names:	3-Decanone Dodecanone-(3) Ethyl nonyl ketone dodecan-3-one
Inchi:	InChI=1S/C12H24O/c1-3-5-6-7-8-9-10-11-12(13)4-2/h3-11H2,1-2H3
InchiKey:	PERIHWAPLOBAJM-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CCCCCCCCC(=O)CC
Mol. weight [g/mol]:	184.32
CAS:	1534-27-6

Physical Properties

Property code	Value	Unit	Source
gf	-78.76	kJ/mol	Joback Method
hf	-403.59	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.106		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1387.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	527.83	K	Joback Method
tc	698.01	K	Joback Method
tf	274.93	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.30	J/molxK	527.83	Joback Method
cpg	452.25	J/molxK	556.19	Joback Method
cpg	467.55	J/molxK	584.56	Joback Method

cpg	482.21	J/molxK	612.92	Joback Method
cpg	496.25	J/molxK	641.28	Joback Method
cpg	509.69	J/molxK	669.65	Joback Method
cpg	522.54	J/molxK	698.01	Joback Method
dvisc	0.0043838	Paxs	274.93	Joback Method
dvisc	0.0019395	Paxs	317.08	Joback Method
dvisc	0.0010391	Paxs	359.23	Joback Method
dvisc	0.0006347	Paxs	401.38	Joback Method
dvisc	0.0004257	Paxs	443.53	Joback Method
dvisc	0.0003061	Paxs	485.68	Joback Method
dvisc	0.0002319	Paxs	527.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52621e+01
Coeff. B	-4.59344e+03
Coeff. C	-8.48900e+01
Temperature range (K), min.	391.64
Temperature range (K), max.	546.51

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1534276&Units=SI>

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
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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