

10-Methyl-2-undecanone

Other names:	10-METHYLUNDECAN-2-ONE
Inchi:	InChI=1S/C12H24O/c1-11(2)9-7-5-4-6-8-10-12(3)13/h11H,4-10H2,1-3H3
InchiKey:	BBBADZRBMLNULE-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CC(=O)CCCCCCCC(C)C
Mol. weight [g/mol]:	184.32
CAS:	---

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
rinpol	1360.00		NIST Webbook
rinpol	1363.00		NIST Webbook
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	452.84	J/mol×K	556.29	Joback Method
cpg	468.47	J/mol×K	585.20	Joback Method
cpg	483.44	J/mol×K	614.10	Joback Method
cpg	497.75	J/mol×K	643.00	Joback Method
cpg	511.43	J/mol×K	671.91	Joback Method

cpg	524.50	J/mol×K	700.81	Joback Method
dvisc	0.0063181	Pa×s	259.93	Joback Method
dvisc	0.0023924	Pa×s	304.51	Joback Method
dvisc	0.0011609	Pa×s	349.08	Joback Method
dvisc	0.0006635	Pa×s	393.66	Joback Method
dvisc	0.0004250	Pa×s	438.24	Joback Method
dvisc	0.0002955	Pa×s	482.81	Joback Method
dvisc	0.0002185	Pa×s	527.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52191e+01
Coeff. B	-4.57634e+03
Coeff. C	-8.47510e+01
Temperature range (K), min.	391.24
Temperature range (K), max.	546.65

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=R508773&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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