

5-Undecanone

Other names:	Butyl hexyl ketone Undecan-5-one
Inchi:	InChI=1S/C11H22O/c1-3-5-7-8-10-11(12)9-6-4-2/h3-10H2,1-2H3
InchiKey:	WENNKWXPawnIOO-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CCCCCCC(=O)CCCC
Mol. weight [g/mol]:	170.29
CAS:	33083-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-87.18	kJ/mol	Joback Method
hf	-382.95	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.716		Crippen Method
mvol	167.420	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rhoc	245.22 ± 6.81	kg/m ³	NIST Webbook
tb	504.95	K	Joback Method
tc	679.40 ± 1.50	K	NIST Webbook
tf	275.00 ± 4.00	K	NIST Webbook
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.23	J/mol×K	504.95	Joback Method
cpg	403.46	J/mol×K	533.52	Joback Method
cpg	418.07	J/mol×K	562.10	Joback Method
cpg	432.09	J/mol×K	590.67	Joback Method
cpg	445.51	J/mol×K	619.25	Joback Method
cpg	458.36	J/mol×K	647.82	Joback Method

cpg	470.65	J/molxK	676.40	Joback Method
dvisc	0.0044945	Paxs	263.66	Joback Method
dvisc	0.0020210	Paxs	303.88	Joback Method
dvisc	0.0010954	Paxs	344.09	Joback Method
dvisc	0.0006749	Paxs	384.30	Joback Method
dvisc	0.0004558	Paxs	424.52	Joback Method
dvisc	0.0003295	Paxs	464.74	Joback Method
dvisc	0.0002508	Paxs	504.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.80	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53084e+01
Coeff. B	-4.46763e+03
Coeff. C	-8.01920e+01
Temperature range (K), min.	377.62
Temperature range (K), max.	527.09

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=C33083839&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/ci9903071
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
rhoc:	Critical density
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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