4-Undecanone

Other names: Heptyl propyl ketone
undecan-4-one
Inchi: InChI=1S/C11H22O/c1-3-5-6-7-8-10-11(12)9-4-2/h3-10H2,1-2H3
InchiKey: NBSLHMOSERBUOV-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCCCCCCC(=O)CCC
Mol. weight [g/mol]: 170.29
CAS: 14476-37-0

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
mcvol	167.420	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rhoc	245.22 ± 6.81	kg/m3	NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1518.00		NIST Webbook
tb	504.95	K	Joback Method
tc	680.90 ± 1.60	K	NIST Webbook
tf	278.00 ± 4.00	K	NIST Webbook
vc	0.657	m3/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/mol×K	676.40	Joback Method
dvisc	0.0044945	Pa×s	263.66	Joback Method
dvisc	0.0020210	Pa×s	303.88	Joback Method
dvisc	0.0010954	Pa×s	344.09	Joback Method
dvisc	0.0006749	Pa×s	384.30	Joback Method
dvisc	0.0004558	Pa×s	424.52	Joback Method
dvisc	0.0003295	Pa×s	464.74	Joback Method
dvisc	0.0002508	Pa×s	504.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60833e+01
Coeff. B	-4.76763e+03
Coeff. C	-8.22700e+01
Temperature range (K), min.	384.10
Temperature range (K), max.	524.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14476370&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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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