5-Decanone

Other names: decan-5-one
Inchi: InChI=1S/C10H20O/c1-3-5-7-9-10(11)8-6-4-2/h3-9H2,1-2H3
InchiKey: JDPQWHLMBJZURR-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCCCCC(=O)CCCC
Mol. weight [g/mol]: 156.27
CAS: 820-29-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.60	kJ/mol	Joback Method
hf	-362.31	kJ/mol	Joback Method
hfus	23.25	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.326		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rhoc	248.46 ± 0.63	kg/m3	NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
tb	477.00 ± 3.00	K	NIST Webbook
tb	477.00 ± 4.00	K	NIST Webbook
tc	661.00 ± 0.40	K	NIST Webbook
tf	263.90 ± 3.00	K	NIST Webbook
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/mol×K	482.07	Joback Method

cpg	356.42	J/mol×K	510.87	Joback Method
cpg	370.27	J/mol×K	539.66	Joback Method
cpg	383.54	J/mol×K	568.46	Joback Method
cpg	396.27	J/mol×K	597.26	Joback Method
cpg	408.46	J/mol×K	626.06	Joback Method
cpg	420.12	J/mol×K	654.85	Joback Method
dvisc	0.0045381	Pa×s	252.39	Joback Method
dvisc	0.0020766	Pa×s	290.67	Joback Method
dvisc	0.0011399	Pa×s	328.95	Joback Method
dvisc	0.0007090	Pa×s	367.23	Joback Method
dvisc	0.0004824	Pa×s	405.51	Joback Method
dvisc	0.0003508	Pa×s	443.79	Joback Method
dvisc	0.0002683	Pa×s	482.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51042e+01
Coeff. B	-4.22821e+03
Coeff. C	-7.37700e+01
Temperature range (K), min.	359.14
Temperature range (K), max.	505.54

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=C820291&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume