OCTYL FORMATE

Other names:	FORMIC ACID,OCTYL ESTER
	Octyl alcohol, formate
	Octyl formiate
	n-Octyl formate
	n-Octyl methanoate
	octyl methanoate
Inchi:	InChI=1S/C9H18O2/c1-2-3-4-5-6-7-8-11-9-10/h9H,2-8H2,1H3
InchiKey:	AVBRYQRTMPHARE-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCCCCCOC=O
Mol. weight [g/mol]:	158.24
CAS:	112-32-3

Physical Properties

Property code	Value	Unit	Source
af	0.6016		Cheméo Relay (1.0)
gf	-179.62	kJ/mol	Joback Method
hf	-494.67	kJ/mol	Cheméo Relay (1.0)
hfus	22.54	kJ/mol	Joback Method
hvap	56.95	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	Cheméo Relay (1.0)
log10ws	-3.45		Cheméo Relay (1.0)
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1128.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1560.00		NIST Webbook
tb	471.30 ± 1.50	K	NIST Webbook
tb	471.95 ± 0.30	K	NIST Webbook

tb	471.00 ± 3.00	K	NIST Webbook
tb	471.95	K	KDB
tc	640.33	K	Cheméo Relay (1.0)
tf	234.05	K	KDB
tf	234.10 ± 0.50	K	NIST Webbook
vc	0.557	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.42	J/mol×K	645.86	Joback Method
cpg	336.68	J/mol×K	504.64	Joback Method
cpg	349.13	J/mol×K	532.89	Joback Method
cpg	323.77	J/mol×K	476.40	Joback Method
cpg	361.12	J/mol×K	561.13	Joback Method
cpg	372.67	J/mol×K	589.37	Joback Method
cpg	383.77	J/mol×K	617.62	Joback Method
dvisc	0.0004563	Pa×s	402.74	Joback Method
dvisc	0.0037595	Pa×s	255.42	Joback Method
dvisc	0.0018180	Pa×s	292.25	Joback Method
dvisc	0.0010344	Pa×s	329.08	Joback Method
dvisc	0.0006593	Pa×s	365.91	Joback Method
dvisc	0.0003359	Pa×s	439.57	Joback Method
dvisc	0.0002592	Pa×s	476.40	Joback Method
pvap	0.06	kPa	303.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.09	kPa	308.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.66	kPa	338.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.49	kPa	333.40	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.43	kPa	331.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.37	kPa	328.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.27	kPa	323.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.19	kPa	318.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.14	kPa	313.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.55	kPa	335.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.01	kPa	283.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.06	kPa	303.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.04	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.02	kPa	290.80	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.02	kPa	288.20	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.02	kPa	285.70	Vapour pressures and enthalpies of vaporization of aliphatic esters

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56616e+01
Coeff. B	-4.40178e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	358.72
Temperature range (K), max.	497.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.89702e+01
Coeff. B	-8.58676e+03
Coeff. C	-9.33680e+00
Coeff. D	5.95103e-06
Temperature range (K), min.	234.05
Temperature range (K), max.	645.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1117

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0):

Vapour pressures and enthalpies of vaporization of aliphatic esters: https://www.doi.org/10.1016/j.fluid.2012.08.003

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112323&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB: https://www.cheric.org/files/research/kdb/mol/mol1117.mol

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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