

Propanoic acid, octyl ester

Other names:	Octyl propanoate Octyl propionate Propionic acid, octyl ester n-Octyl propanoate n-Octyl propionate
Inchi:	InChI=1S/C11H22O2/c1-3-5-6-7-8-9-10-13-11(12)4-2/h3-10H2,1-2H3
InchiKey:	CEQGYPPMTKWBIU-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCCCOC(=O)CC
Mol. weight [g/mol]:	186.29
CAS:	142-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1301.68		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1280.60		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1284.00		NIST Webbook

rinpol	1288.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1542.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1530.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1542.00		NIST Webbook
tb	501.08 ± 0.30	K	NIST Webbook
tb	499.60 ± 1.50	K	NIST Webbook
tc	698.36	K	Joback Method
tf	231.60 ± 0.50	K	NIST Webbook
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.57	J/mol×K	698.36	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	415.24	J/mol×K	527.37	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method
dvisc	0.0015281	Pa×s	326.14	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0002056	Pa×s	527.37	Joback Method

pvap	0.30	kPa	348.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.27	kPa	346.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.21	kPa	343.00	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.18	kPa	340.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.16	kPa	338.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.11	kPa	333.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.08	kPa	328.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.05	kPa	323.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.04	kPa	318.50	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.03	kPa	313.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.02	kPa	308.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.01	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	8.83e-03	kPa	300.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	7.32e-03	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	5.75e-03	kPa	295.70	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	4.65e-03	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56962e+01
Coeff. B	-4.58510e+03
Coeff. C	-8.00530e+01
Temperature range (K), min.	377.62
Temperature range (K), max.	521.58

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142609&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
Vapour pressures and enthalpies of vaporization of aliphatic esters:	https://www.doi.org/10.1016/j.fluid.2012.08.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1128.mol

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/23-786-4/Propanoic-acid-octyl-ester.pdf>

Generated by Cheméo on 2025-12-18 23:04:52.662829307 +0000 UTC m=+5847290.192869971.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.