Butanoic acid, octyl ester

Other names:	Butyric acid, octyl ester
	Octyl butanoate
	Octyl butyrate
	n-Octyl butanoate
	n-Octyl butyrate
	n-Octyl n-butyrate
Inchi:	InChI=1S/C12H24O2/c1-3-5-6-7-8-9-11-14-12(13)10-4-2/h3-11H2,1-2H3
InchiKey:	PWLNAUNEAKQYLH-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCOC(=O)CCC
Mol. weight [g/mol]:	200.32
CAS:	110-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1382.00		NIST Webbook

rinpol	1372.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1620.00		NIST Webbook
tb	506.00 ± 5.00	K	NIST Webbook
tb	515.40 ± 1.50	K	NIST Webbook
tb	244.10 ± 0.50	K	NIST Webbook
tc	720.05	K	Joback Method
tf	217.60 ± 0.50	K	NIST Webbook
tt	218.00	K	Heat capacities of potential organic phase change materials
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method

cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61064e+01
Coeff. B	-4.83744e+03
Coeff. C	-8.49180e+01
Temperature range (K), min.	390.72
Temperature range (K), max.	533.04

Sources

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

Heat capacities of potential organic phase change materials: https://www.doi.org/10.1016/j.jct.2018.08.014

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=C110394&Units=SI

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
tt:	Triple Point Temperature
vc:	Critical Volume