Butanoic acid, hexyl ester

Other names:	1-Hexyl butyrate
	Butyric acid, hexyl ester
	Hexyl butanoate
	Hexyl butyrate
	n-Hexyl butanoate
	n-Hexyl butyrate
	n-Hexyl n-butanoate
	n-Hexyl n-butyrate
Inchi:	InChI=1S/C10H20O2/c1-3-5-6-7-9-12-10(11)8-4-2/h3-9H2,1-2H3
InchiKey:	XAPCMTMQBXLDBB-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCOC(=O)CCC
Mol. weight [g/mol]:	172.26
CAS:	2639-63-6

Physical Properties

Property code	Value	Unit	Source
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1178.00		NIST Webbook
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rinpol	1175.00		NIST Webbook

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rinpol	1174.00	NIST Webbook
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ripol	1424.00		NIST Webbook
ripol	1415.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1426.00		NIST Webbook
tb	478.30 ± 1.50	K	NIST Webbook
tb	481.03 ± 0.30	K	NIST Webbook
tb	478.25 ± 1.00	K	NIST Webbook
tb	466.00 ± 2.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	195.20 ± 0.50	K	NIST Webbook
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.11	J/mol×K	504.49	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	433.67	J/mol×K	648.08	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
dvisc	0.0011310	Pa×s	303.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0012340	Pa×s	298.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0013510	Pa×s	293.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

dvisc	0.0010140	Pa×s	308.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0009610	Pa×s	313.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008890	Pa×s	318.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0008250	Pa×s	323.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007680	Pa×s	328.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0007160	Pa×s	333.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006690	Pa×s	338.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters
dvisc	0.0006270	Pa×s	343.15	Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53031e+01

Coeff. B	-4.30962e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	361.92
Temperature range (K), max.	506.23

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
Density and Viscosity Correlation for Several Common Fragrance and Flavor Esters:	https://www.doi.org/10.1021/je050001c
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=C2639636&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
vc:	Critical Volume

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