Hexanoic acid, butyl ester

Other names:	Butyl caproate
	Butyl ester of hexanoic acid
	Butyl hexanoate
	n-Butyl caproate
	n-Butyl hexanoate
	n-Butyl n-hexanoate
	n-Caproic acid n-butyl ester
Inchi:	InChI=1S/C10H20O2/c1-3-5-7-8-10(11)12-9-6-4-2/h3-9H2,1-2H3
InchiKey:	RPRPDTXKGSIXMD-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCC(=O)OCCCC
Mol. weight [g/mol]:	172.26
CAS:	626-82-4

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	1165.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1190.00		NIST Webbook

rinpol	1156.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1188.00	NIST Webbook
rinpol	1156.00	NIST Webbook
rinpol	1177.00	NIST Webbook
rinpol	1173.00	NIST Webbook
rinpol	1177.00	NIST Webbook
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rinpol	1194.00	NIST Webbook
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ripol	1407.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	480.89 ± 0.30	K	NIST Webbook
tb	477.50 ± 1.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	208.90 ± 0.80	K	NIST Webbook
tf	223.20 ± 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	0.0032806	Pa×s	274.62	Joback Method
dvisc	0.0015931	Pa×s	312.93	Joback Method
dvisc	0.0009057	Pa×s	351.24	Joback Method
dvisc	0.0005753	Pa×s	389.56	Joback Method
dvisc	0.0003964	Pa×s	427.87	Joback Method

dvisc	0.0002904	Pa×s	466.18	Joback Method
dvisc	0.0002230	Pa×s	504.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50661e+01
Coeff. B	-4.24157e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	361.92
Temperature range (K), max.	509.74

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C626824&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

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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