Butanoic acid, 3-methyl-, hexyl ester

Other names:	3-Methylbutanoic acid hexyl ester
	3-Methylbutyric acid hexyl ester
	Hexyl 3-methylbutanoate
	Hexyl 3-methylbutyrate
	Hexyl isopentanoate
	Hexyl isovalerate
	Isovaleric acid, hexyl ester
	n-Hexyl iso-valerate
	n-Hexyl isopentanoate
Inchi:	InChI=1S/C11H22O2/c1-4-5-6-7-8-13-11(12)9-10(2)3/h10H,4-9H2,1-3H3
InchiKey:	RSDDTPVXLMVLQE-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]:	186.29
CAS:	10032-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-194.62	kJ/mol	Joback Method
hf	-520.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.156		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1224.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1204.00		NIST Webbook

rinpol	1243.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1226.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1442.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1457.00		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1450.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	526.93	K	Joback Method
tc	701.19	K	Joback Method
tf	270.89	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/mol×K	526.93	Joback Method
cpg	430.78	J/mol×K	555.97	Joback Method
cpg	445.49	J/mol×K	585.02	Joback Method
cpg	459.60	J/mol×K	614.06	Joback Method
cpg	473.13	J/mol×K	643.11	Joback Method
cpg	486.09	J/mol×K	672.15	Joback Method
cpg	498.48	J/mol×K	701.19	Joback Method

dvisc	0.0044896	Pa×s	270.89	Joback Method
dvisc	0.0018616	Pa×s	313.56	Joback Method
dvisc	0.0009531	Pa×s	356.24	Joback Method
dvisc	0.0005632	Pa×s	398.91	Joback Method
dvisc	0.0003684	Pa×s	441.58	Joback Method
dvisc	0.0002597	Pa×s	484.26	Joback Method
dvisc	0.0001937	Pa×s	526.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46887e+01
Coeff. B	-4.20028e+03
Coeff. C	-7.68560e+01
Temperature range (K), min.	368.52
Temperature range (K), max.	524.78

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10032130&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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