ISOBUTYL HEXANOATE

Other names:	2-Methylpropyl hexanoate
	Hexanoic acid, isobutyl ester
	Isobutyl caproate
	iso-Butyl n-hexanoate
	n-Caproic acid isobutyl ester
Inchi:	InChI=1S/C10H20O2/c1-4-5-6-7-10(11)12-8-9(2)3/h9H,4-8H2,1-3H3
InchiKey:	UXUPPWPIGVTVQI-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	172.27
CAS:	105-79-3

Physical Properties

Property code	Value	Unit	Source
af	0.5890		Cheméo Relay (1.0)
hf	-581.89	kJ/mol	Cheméo Relay (1.0)
hfus	20.92	kJ/mol	Joback Method
hvap	51.80	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1140.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1153.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1131.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1138.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1144.00	NIST Webbook
ripol	1357.00	NIST Webbook
ripol	1356.00	NIST Webbook
ripol	1347.00	NIST Webbook
ripol	1350.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1350.00	NIST Webbook
ripol	1348.00	NIST Webbook
ripol	1399.00	NIST Webbook
ripol	1346.00	NIST Webbook
ripol	1350.00	NIST Webbook
ripol	1346.00	NIST Webbook
ripol	1350.00	NIST Webbook
ripol	1347.00	NIST Webbook
ripol	1346.00	NIST Webbook
ripol	1347.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1351.00	NIST Webbook
ripol	1355.00	NIST Webbook
ripol	1373.00	NIST Webbook
ripol	1353.00	NIST Webbook
ripol	1353.00	NIST Webbook

ripol	1343.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1356.00		NIST Webbook
ripol	1347.00		NIST Webbook
tb	463.25	K	Cheméo Relay (1.0)
tc	637.73	K	Cheméo Relay (1.0)
tf	209.43	K	Cheméo Relay (1.0)
vc	0.609	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/mol×K	504.05	Joback Method
cpg	382.82	J/mol×K	533.34	Joback Method
cpg	396.77	J/mol×K	562.64	Joback Method
cpg	410.17	J/mol×K	591.93	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
dvisc	0.0046674	Pa×s	259.62	Joback Method
dvisc	0.0019627	Pa×s	300.36	Joback Method
dvisc	0.0010151	Pa×s	341.10	Joback Method
dvisc	0.0006043	Pa×s	381.83	Joback Method
dvisc	0.0003976	Pa×s	422.57	Joback Method
dvisc	0.0002816	Pa×s	463.31	Joback Method
dvisc	0.0002109	Pa×s	504.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18714e+01
Coeff. B	-2.99753e+03
Coeff. C	-5.98700e+01
Temperature range (K), min.	318.64
Temperature range (K), max.	516.82

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105793&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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