

Propanoic acid, 2-methyl-, hexyl ester

Other names:	1-Hexyl isobutyrate Hexyl 2-methylpropanoate Hexyl 2-methylpropionate Hexyl isobutanoate Hexyl isobutyrate Isobutyric acid, hexyl ester NSC 46108 n-Hexyl isobutanoate n-Hexyl isobutyrate
Inchi:	InChI=1S/C10H20O2/c1-4-5-6-7-8-12-10(11)9(2)3/h9H,4-8H2,1-3H3
InchiKey:	CYHBDKTZDLSEMY-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCOC(=O)C(C)C
Mol. weight [g/mol]:	172.26
CAS:	2349-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-203.04	kJ/mol	Joback Method
hf	-499.81	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1145.20		NIST Webbook
rinpol	1148.50		NIST Webbook

rinpol	1132.00	NIST Webbook
rinpol	1131.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1151.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1147.00	NIST Webbook
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rinpol	1135.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1152.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1117.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1145.20	NIST Webbook
rinpol	1132.00	NIST Webbook
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rinpol	1117.00	NIST Webbook
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ripol	1335.00	NIST Webbook
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ripol	1350.00	NIST Webbook
ripol	1335.00	NIST Webbook

ripol	1331.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1337.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1333.00		NIST Webbook
tb	472.00 ± 3.00	K	NIST Webbook
tc	679.81	K	Joback Method
tf	259.62	K	Joback Method
vc	0.614	m3/kmol	Joback Method

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	381.84	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47536e+01
Coeff. B	-4.09086e+03
Coeff. C	-7.21300e+01
Temperature range (K), min.	354.92
Temperature range (K), max.	505.38

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2349077&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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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