

Formic acid, hexyl ester

Other names:	Hexyl formate Hexyl formiate hexyl methanoate methanoic acid, hexyl ester n-Hexyl formate n-Hexyl methanoate
Inchi:	InChI=1S/C7H14O2/c1-2-3-4-5-6-9-7-8/h7H,2-6H2,1H3
InchiKey:	OUGPMNMLWKSBI-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CCCCCCOC=O
Mol. weight [g/mol]:	130.18
CAS:	629-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-196.46	kJ/mol	Joback Method
hf	-405.61	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.740		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	870.00		NIST Webbook

rinpol	884.00		NIST Webbook
rinpol	907.00		NIST Webbook
ripol	1382.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1347.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1371.00		NIST Webbook
tb	426.80 ± 1.50	K	NIST Webbook
tb	428.66 ± 0.30	K	NIST Webbook
tb	427.00 ± 2.00	K	NIST Webbook
tb	427.00 ± 2.00	K	NIST Webbook
tb	428.66	K	KDB
tb	419.00 ± 1.00	K	NIST Webbook
tc	602.36	K	Joback Method
tf	210.50 ± 0.30	K	NIST Webbook
tf	210.50	K	KDB
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.14	J/mol×K	430.64	Joback Method
cpg	261.33	J/mol×K	487.88	Joback Method
cpg	271.39	J/mol×K	516.50	Joback Method
cpg	281.10	J/mol×K	545.12	Joback Method
cpg	290.46	J/mol×K	573.74	Joback Method
cpg	299.47	J/mol×K	602.36	Joback Method
cpg	250.91	J/mol×K	459.26	Joback Method
dvisc	0.0018090	Paxs	265.84	Joback Method
dvisc	0.0010617	Paxs	298.80	Joback Method
dvisc	0.0006927	Paxs	331.76	Joback Method
dvisc	0.0004882	Paxs	364.72	Joback Method
dvisc	0.0003646	Paxs	397.68	Joback Method
dvisc	0.0035841	Paxs	232.88	Joback Method
dvisc	0.0002848	Paxs	430.64	Joback Method
pvap	1.01	kPa	313.40	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	1.02	kPa	313.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.76	kPa	308.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.75	kPa	308.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.54	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.56	kPa	303.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.41	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.41	kPa	298.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.28	kPa	293.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.27	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.19	kPa	288.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.13	kPa	283.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.09	kPa	278.50	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.07	kPa	275.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56395e+01
Coeff. B	-4.04284e+03
Coeff. C	-6.01760e+01
Temperature range (K), min.	323.52
Temperature range (K), max.	451.62

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629334&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of aliphatic esters:	https://www.doi.org/10.1016/j.fluid.2012.08.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1095.mol
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

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