Hexanoic acid, hexyl ester

Other names:	Hexyl caproate
	Hexyl hexanoate
	Hexyl hexoate
	Hexyl n-hexanoate
	n-Hexyl caproate
	n-Hexyl hexanoate
	n-Hexyl n-hexanoate
Inchi:	InChI=1S/C12H24O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h3-11H2,1-2H3
InchiKey:	NCDCLPBOMHPFCV-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	200.32
CAS:	6378-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1383.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1392.00		NIST Webbook

rinpol	1371.00	NIST Webbook
rinpol	1383.00	NIST Webbook
rinpol	1392.00	NIST Webbook
rinpol	1386.00	NIST Webbook
rinpol	1394.00	NIST Webbook
rinpol	1370.00	NIST Webbook
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rinpol	1379.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1370.00	NIST Webbook
rinpol	1371.00	NIST Webbook
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rinpol	1376.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1373.00	NIST Webbook
rinpol	1367.00	NIST Webbook
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ripol	1608.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1617.00		NIST Webbook
tb	518.58 ± 0.30	K	NIST Webbook
tc	720.05	K	Joback Method
tf	217.90 ± 0.40	K	NIST Webbook
tt	217.00	K	Heat capacities of potential organic phase change materials
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.22	J/mol×K	720.05	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	464.17	J/mol×K	550.25	Joback Method

dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method
pvap	3.13e-03	kPa	298.40	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	4.90e-03	kPa	303.20	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	7.32e-03	kPa	308.00	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.01	kPa	312.80	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.01	kPa	312.80	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.02	kPa	317.70	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.03	kPa	322.60	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.04	kPa	327.50	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

pvap	0.05	kPa	332.40	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.08	kPa	337.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.11	kPa	342.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.14	kPa	347.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction
pvap	0.15	kPa	347.30	Biomass Valorization: Thermodynamics of the Guerbet Condensation Reaction

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51432e+01
Coeff. B	-4.55839e+03
Coeff. C	-8.54740e+01
Temperature range (K), min.	392.32
Temperature range (K), max.	549.11

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6378650&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
Heat capacities of potential organic phase change materials:	https://www.doi.org/10.1016/j.jct.2018.08.014
Biomass Valorization:	https://www.doi.org/10.1021/acs.jced.9b00419
Thermodynamics of the Guerbet Condensation Reaction:	https://en.wikipedia.org/wiki/Joback_method
Joback Method:	

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
tt:	Triple Point Temperature
vc:	Critical Volume