HEXYL PENTANOATE

Other names:	1-Hexyl n-valerate
	Hexyl n-valerate
	Hexyl valerate
	Hexyl valerianate
	Pentanoic acid, hexyl ester
	Valeric acid, hexyl ester
Inchi:	InChI=1S/C11H22O2/c1-3-5-7-8-10-13-11(12)9-6-4-2/h3-10H2,1-2H3
InchiKey:	YERFHJZYNMRVLO-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	186.30
CAS:	1117-59-5

Physical Properties

Property code	Value	Unit	Source
af	0.6578		Cheméo Relay (1.0)
gf	-192.18	kJ/mol	Joback Method
hf	-592.07	kJ/mol	Cheméo Relay (1.0)
hfus	27.03	kJ/mol	Joback Method
hvap	59.19	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-3.55		Cheméo Relay (1.0)
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1266.00		NIST Webbook

rinpol	1235.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1502.00		NIST Webbook
tb	499.45 ± 0.30	K	NIST Webbook
tb	497.00 ± 2.00	K	NIST Webbook
tc	669.65	K	Cheméo Relay (1.0)
tf	210.10 ± 0.50	K	NIST Webbook
vc	0.672	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.24	J/mol×K	527.37	Joback Method
cpg	496.57	J/mol×K	698.36	Joback Method
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0002056	Pa×s	527.37	Joback Method
dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0015281	Pa×s	326.14	Joback Method

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55591e+01
Coeff. B	-4.52897e+03
Coeff. C	-7.99970e+01
Temperature range (K), min.	376.56
Temperature range (K), max.	521.95

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1127.mol
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=C1117595&Units=SI
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):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
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