Heptane, 3-(chloromethyl)-

Other names:	1-Chloro-2-ethylhexane
	2-Ethylhexyl chloride
	3-(Chloromethyl)heptane
	hexane, 1-chloro-2-ethyl-
Inchi:	InChI=1S/C8H17Cl/c1-3-5-6-8(4-2)7-9/h8H,3-7H2,1-2H3
InchiKey:	WLVCBAMXYMWGLJ-UHFFFAOYSA-N
Formula:	C8H17Cl
SMILES:	CCCCC(CC)CCl
Mol. weight [g/mol]:	148.67
CAS:	123-04-6

Physical Properties

Property code	Value	Unit	Source
gf	2.11	kJ/mol	Joback Method
hf	-229.47	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.442		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	445.40	K	Isobaric Vapor Liquid Equilibria for Binary Systems Comprising 1-Chloro-2-ethylhexane, 2-Ethyl-1-hexanol, p-Xylene, and N-Methylpyrrolidone (NMP) at 40.0 kPa
tc	594.11	K	Joback Method
tf	194.84	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	312.27	J/mol×K	535.88	Joback Method
cpg	334.03	J/mol×K	594.11	Joback Method
cpg	323.39	J/mol×K	564.99	Joback Method
cpg	262.83	J/mol×K	419.43	Joback Method
cpg	275.97	J/mol×K	448.54	Joback Method
cpg	288.58	J/mol×K	477.66	Joback Method
cpg	300.68	J/mol×K	506.77	Joback Method
dvisc	0.0002677	Pa×s	419.43	Joback Method
dvisc	0.0005177	Pa×s	344.57	Joback Method
dvisc	0.0003605	Pa×s	382.00	Joback Method
dvisc	0.0088497	Pa×s	194.84	Joback Method
dvisc	0.0030882	Pa×s	232.27	Joback Method
dvisc	0.0014434	Pa×s	269.70	Joback Method
dvisc	0.0008121	Pa×s	307.13	Joback Method
hvapt	44.20	kJ/mol	407.00	NIST Webbook
rfi	1.43260		293.10	Vapor-Liquid Equilibria of Binary Systems Comprising 1-Chloro-2-ethylhexane and 2-Ethyl-1-hexanol
rfi	1.43260		293.10	Phase Equilibria of Binary Systems Comprising Formic Acid, N,N-Dimethylformamide, 1-Chloro-2-ethylhexane, and 2-Ethyl-1-hexanol

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48971e+01
Coeff. B	-3.97698e+03
Coeff. C	-6.49020e+01
Temperature range (K), min.	337.12
Temperature range (K), max.	479.79

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123046&Units=SI
Vapor-Liquid Equilibria of Binary Systems Comprising 1-Chloro-2-ethylhexane and 2-Ethyl-1-hexanol, N,N-Dimethylformamide, Formic Acid, Isobutyric Acid, and N-Methylpyrrolidone (NMP) at 40.0 kPa:	https://www.doi.org/10.1021/je8001249
Phase Equilibria of Binary Systems Comprising 1-Chloro-2-ethylhexane and 2-Ethyl-1-hexanol:	https://www.doi.org/10.1021/je800123c
Isobaric Vapor-Liquid Equilibria for Binary Systems Comprising 1-Chloro-2-ethylhexane and 2-Ethyl-1-hexanol:	https://www.doi.org/10.1021/je300848z
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
1-Chloro-2-ethylhexane, 2-Ethyl-1-hexanol, p-Xylene, and N-Methylpyrrolidone (NMP) at 40.0 kPa:	http://link.springer.com/article/10.1007/BF02311772
McGowan 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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume