Hexanoyl chloride, 2-ethyl-

Other names:	2-Ethylhexanoic acid, chloride
	2-Ethylhexanoyl chloride
	2-Ethylcaproic acid chloride
	2-Ethylcaproyl chloride
Inchi:	InChI=1S/C8H15ClO/c1-3-5-6-7(4-2)8(9)10/h7H,3-6H2,1-2H3
InchiKey:	WFSGQBNCVASPMW-UHFFFAOYSA-N
Formula:	C8H15ClO
SMILES:	CCCCC(CC)C(=O)Cl
Mol. weight [g/mol]:	162.66
CAS:	760-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-126.81	kJ/mol	Joback Method
hf	-342.05	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.968		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1040.00		NIST Webbook
tb	473.30	K	Joback Method
tc	658.88	K	Joback Method
tf	244.77	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.06	J/mol×K	473.30	Joback Method
cpg	340.74	J/mol×K	627.95	Joback Method
cpg	330.46	J/mol×K	597.02	Joback Method
cpg	319.66	J/mol×K	566.09	Joback Method

cpg	308.34	J/mol×K	535.16	Joback Method
cpg	296.48	J/mol×K	504.23	Joback Method
cpg	350.53	J/mol×K	658.88	Joback Method
dvisc	0.0003000	Pa×s	473.30	Joback Method
dvisc	0.0003972	Pa×s	435.21	Joback Method
dvisc	0.0005552	Pa×s	397.12	Joback Method
dvisc	0.0008331	Pa×s	359.03	Joback Method
dvisc	0.0013764	Pa×s	320.95	Joback Method
dvisc	0.0026033	Pa×s	282.86	Joback Method
dvisc	0.0060041	Pa×s	244.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.70	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C760678&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume