2-ETHYLHEXANOYL CHLORIDE

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

Physical Properties

Property code	Value	Unit	Source
af	0.4524		Cheméo Relay (1.0)
hf	-362.01	kJ/mol	Cheméo Relay (1.0)
hfus	18.75	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-3.31		Cheméo Relay (1.0)
logp	2.968		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1040.00		NIST Webbook
tb	448.69	K	Cheméo Relay (1.0)
tc	628.31	K	Cheméo Relay (1.0)
tf	175.53	K	Cheméo Relay (1.0)
vc	0.486	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.06	J/mol×K	473.30	Joback Method
cpg	296.48	J/mol×K	504.23	Joback Method
cpg	308.34	J/mol×K	535.16	Joback Method
cpg	319.66	J/mol×K	566.09	Joback Method

cpg	330.46	J/mol×K	597.02	Joback Method
cpg	340.74	J/mol×K	627.95	Joback Method
cpg	350.53	J/mol×K	658.88	Joback Method
dvisc	0.0060041	Pa×s	244.77	Joback Method
dvisc	0.0026033	Pa×s	282.86	Joback Method
dvisc	0.0013764	Pa×s	320.95	Joback Method
dvisc	0.0008331	Pa×s	359.03	Joback Method
dvisc	0.0005552	Pa×s	397.12	Joback Method
dvisc	0.0003972	Pa×s	435.21	Joback Method
dvisc	0.0003000	Pa×s	473.30	Joback Method

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C760678&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
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