(2E)-2-butenoyl chloride

Other names:	Crotonyl chloride
	Crotonic acid chloride
	(2E)-2-butenoyl chloride
	crotonoyl chloride
Inchi:	InChI=1S/C4H5ClO/c1-2-3-4(5)6/h2-3H,1H3
InchiKey:	RJUIDDKTATZJFE-UHFFFAOYSA-N
Formula:	C4H5ClO
SMILES:	CC=CC(=O)Cl
Mol. weight [g/mol]:	104.54

Physical Properties

Property code	Value	Unit	Source
hf	-173.31	kJ/mol	Cheméo Relay (1.0)
hfus	12.11	kJ/mol	Joback Method
hvap	34.47	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-1.29		Cheméo Relay (1.0)
logp	1.328		Crippen Method
mcvol	76.730	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	796.00		NIST Webbook
tb	394.00 ± 4.00	K	NIST Webbook
tb	394.00 ± 4.00	K	NIST Webbook
tc	581.73	K	Cheméo Relay (1.0)
tf	201.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.29	J/mol×K	386.38	Joback Method
cpg	150.21	J/mol×K	584.10	Joback Method
cpg	145.38	J/mol×K	551.15	Joback Method
cpg	140.25	J/mol×K	518.20	Joback Method
cpg	134.79	J/mol×K	485.24	Joback Method

cpg	128.99	J/mol×K	452.29	Joback Method
cpg	122.83	J/mol×K	419.33	Joback Method
dvisc	0.0006807	Pa×s	298.00	Joback Method
dvisc	0.0002969	Pa×s	386.38	Joback Method
dvisc	0.0003740	Pa×s	356.92	Joback Method
dvisc	0.0004911	Pa×s	327.46	Joback Method
dvisc	0.0031414	Pa×s	209.61	Joback Method
dvisc	0.0010133	Pa×s	268.53	Joback Method
dvisc	0.0016640	Pa×s	239.07	Joback Method

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10487715&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

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
tc: Critical Temperature
tf: Normal melting (fusion) point

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