4-CHLOROBUTYRYL CHLORIDE

Other names:	«gamma»-Chlorobutyryl chloride
	4-Chlorobutyryl chloride
	4-Chlorobutyl chloride
	«gamma»-Chloro-n-butyryl chloride
	4-Chlorobutyroyl chloride
Inchi:	InChI=1S/C4H6Cl2O/c5-3-1-2-4(6)7/h1-3H2
InchiKey:	CDIIZULDSLKBKV-UHFFFAOYSA-N
Formula:	C4H6Cl2O
SMILES:	O=C(Cl)CCCCl
Mol. weight [g/mol]:	141.00

Physical Properties

Property code	Value	Unit	Source
hf	-290.20	kJ/mol	Cheméo Relay (1.0)
hfus	16.11	kJ/mol	Joback Method
hvap	43.00	kJ/mol	Cheméo Relay (1.0)
ie	10.48	eV	Cheméo Relay (1.0)
logp	1.771		Crippen Method
mcvol	93.270	ml/mol	McGowan Method
rinpol	959.70		NIST Webbook
tb	446.70	K	NIST Webbook
tf	233.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.74	J/mol×K	419.65	Joback Method
cpg	159.49	J/mol×K	452.22	Joback Method
cpg	165.90	J/mol×K	484.79	Joback Method
cpg	172.00	J/mol×K	517.37	Joback Method
cpg	177.79	J/mol×K	549.94	Joback Method
cpg	183.28	J/mol×K	582.51	Joback Method
cpg	188.48	J/mol×K	615.08	Joback Method
dvisc	0.0036532	Pa×s	244.61	Joback Method

dvisc	0.0020955	Pa×s	273.78	Joback Method
dvisc	0.0013378	Pa×s	302.96	Joback Method
dvisc	0.0009241	Pa×s	332.13	Joback Method
dvisc	0.0006777	Pa×s	361.30	Joback Method
dvisc	0.0005205	Pa×s	390.48	Joback Method
dvisc	0.0004147	Pa×s	419.65	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4635590&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

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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point