

Butanoyl chloride

Other names:	Butyryl chloride n-Butyryl chloride Butyric acid chloride Butyric chloride n-Butyric acid chloride UN 2353
Inchi:	InChI=1S/C4H7ClO/c1-2-3-4(5)6/h2-3H2,1H3
InchiKey:	DVECBJCOGJRVPX-UHFFFAOYSA-N
Formula:	C4H7ClO
SMILES:	CCCC(=O)Cl
Mol. weight [g/mol]:	106.55
CAS:	141-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-158.05	kJ/mol	Joback Method
hf	-254.21	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.552		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	705.00		NIST Webbook
rinpol	709.10		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	709.10		NIST Webbook
tb	375.00 ± 0.60	K	NIST Webbook
tb	375.00	K	NIST Webbook
tb	377.00 ± 8.00	K	NIST Webbook
tb	375.20	K	NIST Webbook
tb	374.70 ± 1.00	K	NIST Webbook
tc	569.79	K	Joback Method
tf	184.20 ± 1.00	K	NIST Webbook
tf	184.20 ± 0.60	K	NIST Webbook
vc	0.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.57	J/molxK	382.22	Joback Method
cpg	138.59	J/molxK	413.48	Joback Method
cpg	145.30	J/molxK	444.74	Joback Method
cpg	151.74	J/molxK	476.01	Joback Method
cpg	157.89	J/molxK	507.27	Joback Method
cpg	163.76	J/molxK	538.53	Joback Method
cpg	169.37	J/molxK	569.79	Joback Method
cpl	170.70	J/molxK	298.00	NIST Webbook
dvisc	0.0034502	Paxs	214.69	Joback Method
dvisc	0.0019085	Paxs	242.61	Joback Method
dvisc	0.0011929	Paxs	270.53	Joback Method
dvisc	0.0008142	Paxs	298.46	Joback Method
dvisc	0.0005932	Paxs	326.38	Joback Method
dvisc	0.0004543	Paxs	354.30	Joback Method
dvisc	0.0003618	Paxs	382.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141753&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvac:	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
rinqol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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