

4-Chlorobutanoic anhydride

Inchi:	InChI=1S/C8H12Cl2O3/c9-5-1-3-7(11)13-8(12)4-2-6-10/h1-6H2
InchiKey:	VAXCCWFPTAPDMK-UHFFFAOYSA-N
Formula:	C8H12Cl2O3
SMILES:	O=C(CCCCl)OC(=O)CCCl
Mol. weight [g/mol]:	227.09

Physical Properties

Property code	Value	Unit	Source
gf	-370.22	kJ/mol	Joback Method
hf	-597.31	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.094		Crippen Method
mcvol	157.070	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinqol	1596.70		NIST Webbook
tb	587.46	K	Joback Method
tc	781.58	K	Joback Method
tf	361.85	K	Joback Method
vc	0.612	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.34	J/molxK	587.46	Joback Method
cpg	396.47	J/molxK	749.23	Joback Method
cpg	388.07	J/molxK	716.88	Joback Method
cpg	379.16	J/molxK	684.52	Joback Method
cpg	369.74	J/molxK	652.17	Joback Method
cpg	359.80	J/molxK	619.81	Joback Method
cpg	404.37	J/molxK	781.58	Joback Method
dvisc	0.0002626	Paxs	587.46	Joback Method
dvisc	0.0003323	Paxs	549.86	Joback Method

dvisc	0.0004352	Paxs	512.26	Joback Method
dvisc	0.0005949	Paxs	474.66	Joback Method
dvisc	0.0008580	Paxs	437.05	Joback Method
dvisc	0.0013259	Paxs	399.45	Joback Method
dvisc	0.0022430	Paxs	361.85	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=U333911&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/31-595-7/4-Chlorobutanoic-anhydride.pdf>

Generated by Cheméo on 2024-04-24 20:56:25.997390694 +0000 UTC m=+16281434.917968007.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.