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)CCCCl
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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.34	J/mol×K	587.46	Joback Method
cpg	359.80	J/mol×K	619.81	Joback Method
cpg	369.74	J/mol×K	652.17	Joback Method
cpg	379.16	J/mol×K	684.52	Joback Method
cpg	388.07	J/mol×K	716.88	Joback Method
cpg	396.47	J/mol×K	749.23	Joback Method
cpg	404.37	J/mol×K	781.58	Joback Method
dvisc	0.0022430	Pa×s	361.85	Joback Method
dvisc	0.0013259	Pa×s	399.45	Joback Method

dvisc	0.0008580	Pa×s	437.05	Joback Method
dvisc	0.0005949	Pa×s	474.66	Joback Method
dvisc	0.0004352	Pa×s	512.26	Joback Method
dvisc	0.0003323	Pa×s	549.86	Joback Method
dvisc	0.0002626	Pa×s	587.46	Joback Method

Sources

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

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