

Carbonic acid, 2-chloroethyl cyclohexyl ester

Inchi:	InChI=1S/C9H15ClO3/c10-6-7-12-9(11)13-8-4-2-1-3-5-8/h8H,1-7H2
InchiKey:	IJDRTYIIAPJELW-UHFFFAOYSA-N
Formula:	C9H15ClO3
SMILES:	O=C(OCCCl)OC1CCCCC1
Mol. weight [g/mol]:	206.67

Physical Properties

Property code	Value	Unit	Source
gf	-301.50	kJ/mol	Joback Method
hf	-567.53	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.711		Crippen Method
mcvol	152.360	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinsol	1463.00		NIST Webbook
tb	561.01	K	Joback Method
tc	772.14	K	Joback Method
tf	322.88	K	Joback Method
vc	0.564	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.35	J/molxK	561.01	Joback Method
cpg	380.23	J/molxK	596.20	Joback Method
cpg	395.29	J/molxK	631.39	Joback Method
cpg	409.51	J/molxK	666.57	Joback Method
cpg	422.91	J/molxK	701.76	Joback Method
cpg	435.48	J/molxK	736.95	Joback Method
cpg	447.21	J/molxK	772.14	Joback Method
dvisc	0.0026756	Paxs	322.88	Joback Method
dvisc	0.0013843	Paxs	362.57	Joback Method

dvisc	0.0008156	Paxs	402.26	Joback Method
dvisc	0.0005285	Paxs	441.94	Joback Method
dvisc	0.0003678	Paxs	481.63	Joback Method
dvisc	0.0002705	Paxs	521.32	Joback Method
dvisc	0.0002078	Paxs	561.01	Joback Method

Sources

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=U357880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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