

Carbonic acid, 2-chloroethyl cyclohexylmethyl ester

Inchi:	InChI=1S/C10H17ClO3/c11-6-7-13-10(12)14-8-9-4-2-1-3-5-9/h9H,1-8H2
InchiKey:	ZVBGRKZOGKOZEI-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	O=C(OCCCl)OCC1CCCCC1
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-293.08	kJ/mol	Joback Method
hf	-588.17	kJ/mol	Joback Method
hfus	21.66	kJ/mol	Joback Method
hvap	54.23	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.959		Crippen Method
mvol	166.450	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	583.89	K	Joback Method
tc	791.65	K	Joback Method
tf	334.15	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.15	J/molxK	583.89	Joback Method
cpg	429.73	J/molxK	618.52	Joback Method
cpg	445.43	J/molxK	653.14	Joback Method
cpg	460.25	J/molxK	687.77	Joback Method
cpg	474.19	J/molxK	722.39	Joback Method
cpg	487.27	J/molxK	757.02	Joback Method
cpg	499.47	J/molxK	791.65	Joback Method
dvisc	0.0025335	Paxs	334.15	Joback Method

dvisc	0.0012892	Paxs	375.77	Joback Method
dvisc	0.0007507	Paxs	417.40	Joback Method
dvisc	0.0004821	Paxs	459.02	Joback Method
dvisc	0.0003333	Paxs	500.64	Joback Method
dvisc	0.0002439	Paxs	542.27	Joback Method
dvisc	0.0001865	Paxs	583.89	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=U357883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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