

Carbonic acid, 2-chloroethyl phenyl ester

Inchi:	InChI=1S/C9H9ClO3/c10-6-7-12-9(11)13-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	WJEJDRWBQAGQIY-UHFFFAOYSA-N
Formula:	C9H9ClO3
SMILES:	O=C(OCCCl)Oc1ccccc1
Mol. weight [g/mol]:	200.62

Physical Properties

Property code	Value	Unit	Source
gf	-213.54	kJ/mol	Joback Method
hf	-385.32	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	53.86	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.441		Crippen Method
mvol	139.460	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1484.00		NIST Webbook
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tb	568.14	K	Joback Method
tc	786.49	K	Joback Method
tf	341.92	K	Joback Method
vc	0.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.13	J/molxK	568.14	Joback Method
cpg	315.77	J/molxK	604.53	Joback Method
cpg	326.74	J/molxK	640.92	Joback Method
cpg	337.03	J/molxK	677.32	Joback Method
cpg	346.66	J/molxK	713.71	Joback Method
cpg	355.62	J/molxK	750.10	Joback Method
cpg	363.91	J/molxK	786.49	Joback Method
dvisc	0.0016397	Paxs	341.92	Joback Method

dvisc	0.0009572	Paxs	379.62	Joback Method
dvisc	0.0006159	Paxs	417.33	Joback Method
dvisc	0.0004263	Paxs	455.03	Joback Method
dvisc	0.0003122	Paxs	492.73	Joback Method
dvisc	0.0002390	Paxs	530.44	Joback Method
dvisc	0.0001895	Paxs	568.14	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=U357881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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