

Carbonic acid, 2-chloroethyl neopentyl ester

Inchi:	InChI=1S/C8H15ClO3/c1-8(2,3)6-12-7(10)11-5-4-9/h4-6H2,1-3H3
InchiKey:	NYIQAUKWXYWVSR-UHFFFAOYSA-N
Formula:	C8H15ClO3
SMILES:	CC(C)(C)COC(=O)OCCCI
Mol. weight [g/mol]:	194.66

Physical Properties

Property code	Value	Unit	Source
gf	-331.53	kJ/mol	Joback Method
hf	-609.96	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.425		Crippen Method
mcvol	149.130	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1194.00		NIST Webbook
tb	515.35	K	Joback Method
tc	706.00	K	Joback Method
tf	306.65	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.76	J/mol×K	515.35	Joback Method
cpg	391.92	J/mol×K	674.22	Joback Method
cpg	381.61	J/mol×K	642.45	Joback Method
cpg	370.75	J/mol×K	610.67	Joback Method
cpg	359.33	J/mol×K	578.90	Joback Method
cpg	347.34	J/mol×K	547.12	Joback Method
cpg	401.68	J/mol×K	706.00	Joback Method
dvisc	0.0002037	Pa×s	515.35	Joback Method
dvisc	0.0002684	Pa×s	480.57	Joback Method

dvisc	0.0003694	Pa×s	445.78	Joback Method
dvisc	0.0005365	Pa×s	411.00	Joback Method
dvisc	0.0008349	Pa×s	376.22	Joback Method
dvisc	0.0014218	Pa×s	341.43	Joback Method
dvisc	0.0027321	Pa×s	306.65	Joback Method

Sources

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=U357877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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