

Carbonic acid, 2-chloroethyl 2-ethylhexyl ester

Inchi:	InChI=1S/C11H21ClO3/c1-3-5-6-10(4-2)9-15-11(13)14-8-7-12/h10H,3-9H2,1-2H3
InchiKey:	VHIUMWYSMUNWJU-UHFFFAOYSA-N
Formula:	C11H21ClO3
SMILES:	CCCCC(CC)COC(=O)OCCCI
Mol. weight [g/mol]:	236.74

Physical Properties

Property code	Value	Unit	Source
gf	-311.55	kJ/mol	Joback Method
hf	-668.41	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.595		Crippen Method
mcvol	191.400	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1535.00		NIST Webbook
tb	586.78	K	Joback Method
tc	765.18	K	Joback Method
tf	323.04	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.59	J/molxK	586.78	Joback Method
cpg	488.08	J/molxK	616.51	Joback Method
cpg	501.97	J/molxK	646.25	Joback Method
cpg	515.26	J/molxK	675.98	Joback Method
cpg	527.95	J/molxK	705.71	Joback Method
cpg	540.05	J/molxK	735.45	Joback Method
cpg	551.55	J/molxK	765.18	Joback Method
dvisc	0.0025229	Paxs	323.04	Joback Method
dvisc	0.0011816	Paxs	367.00	Joback Method

dvisc	0.0006509	Paxs	410.95	Joback Method
dvisc	0.0004024	Paxs	454.91	Joback Method
dvisc	0.0002707	Paxs	498.87	Joback Method
dvisc	0.0001942	Paxs	542.82	Joback Method
dvisc	0.0001465	Paxs	586.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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