

8-Chlorooctyl ethyl carbonate

Inchi:	InChI=1S/C11H21ClO3/c1-2-14-11(13)15-10-8-6-4-3-5-7-9-12/h2-10H2,1H3
InchiKey:	SWQKLBIZVFJKQV-UHFFFAOYSA-N
Formula:	C11H21ClO3
SMILES:	CCOC(=O)OCCCCCCCCI
Mol. weight [g/mol]:	236.74

Physical Properties

Property code	Value	Unit	Source
gf	-309.11	kJ/mol	Joback Method
hf	-663.13	kJ/mol	Joback Method
hfus	32.42	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.739		Crippen Method
mvol	191.400	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	587.22	K	Joback Method
tc	762.56	K	Joback Method
tf	338.04	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.22	J/molxK	587.22	Joback Method
cpg	487.41	J/molxK	616.44	Joback Method
cpg	501.03	J/molxK	645.67	Joback Method
cpg	514.08	J/molxK	674.89	Joback Method
cpg	526.56	J/molxK	704.11	Joback Method
cpg	538.47	J/molxK	733.34	Joback Method
cpg	549.81	J/molxK	762.56	Joback Method
dvisc	0.0019474	Paxs	338.04	Joback Method

dvisc	0.0010168	Paxs	379.57	Joback Method
dvisc	0.0006035	Paxs	421.10	Joback Method
dvisc	0.0003933	Paxs	462.63	Joback Method
dvisc	0.0002751	Paxs	504.16	Joback Method
dvisc	0.0002032	Paxs	545.69	Joback Method
dvisc	0.0001566	Paxs	587.22	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=U373785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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