

Carbonic acid, 2,2,2-trichloroethyl 2-ethylhexyl ester

Inchi:	InChI=1S/C11H19Cl3O3/c1-3-5-6-9(4-2)7-16-10(15)17-8-11(12,13)14/h9H,3-8H2,1-2H3
InchiKey:	LBTHIGOEGLDVVOW-UHFFFAOYSA-N
Formula:	C11H19Cl3O3
SMILES:	CCCCC(CC)COC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	305.63

Physical Properties

Property code	Value	Unit	Source
gf	-332.57	kJ/mol	Joback Method
hf	-708.64	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.726		Crippen Method
mvol	215.880	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	1691.00		NIST Webbook
tb	658.41	K	Joback Method
tc	854.29	K	Joback Method
tf	385.30	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.07	J/molxK	658.41	Joback Method
cpg	547.55	J/molxK	691.06	Joback Method
cpg	560.26	J/molxK	723.70	Joback Method
cpg	572.22	J/molxK	756.35	Joback Method
cpg	583.44	J/molxK	789.00	Joback Method
cpg	593.94	J/molxK	821.64	Joback Method
cpg	603.76	J/molxK	854.29	Joback Method
dvisc	0.0017317	Paxs	385.30	Joback Method
dvisc	0.0008422	Paxs	430.82	Joback Method

dvisc	0.0004701	Paxs	476.34	Joback Method
dvisc	0.0002905	Paxs	521.86	Joback Method
dvisc	0.0001939	Paxs	567.37	Joback Method
dvisc	0.0001374	Paxs	612.89	Joback Method
dvisc	0.0001022	Paxs	658.41	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=U357897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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