

Carbonic acid, 2,2,2-trichloroethyl 2-pentyl ester

Inchi:	InChI=1S/C8H13Cl3O3/c1-3-4-6(2)14-7(12)13-5-8(9,10)11/h6H,3-5H2,1-2H3
InchiKey:	QHFGYKUQJJHXDS-UHFFFAOYSA-N
Formula:	C8H13Cl3O3
SMILES:	CCCC(C)OC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	263.55

Physical Properties

Property code	Value	Unit	Source
gf	-357.83	kJ/mol	Joback Method
hf	-646.72	kJ/mol	Joback Method
hfus	22.10	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.698		Crippen Method
mvol	173.610	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1383.00		NIST Webbook
tb	589.77	K	Joback Method
tc	793.61	K	Joback Method
tf	351.49	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.17	J/molxK	589.77	Joback Method
cpg	438.13	J/molxK	759.64	Joback Method
cpg	429.21	J/molxK	725.66	Joback Method
cpg	419.67	J/molxK	691.69	Joback Method
cpg	409.49	J/molxK	657.72	Joback Method
cpg	398.66	J/molxK	623.74	Joback Method
cpg	446.46	J/molxK	793.61	Joback Method
dvisc	0.0001578	Paxs	589.77	Joback Method
dvisc	0.0002103	Paxs	550.06	Joback Method

dvisc	0.0002931	Paxs	510.34	Joback Method
dvisc	0.0004320	Paxs	470.63	Joback Method
dvisc	0.0006840	Paxs	430.92	Joback Method
dvisc	0.0011888	Paxs	391.20	Joback Method
dvisc	0.0023411	Paxs	351.49	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357894&Units=SI

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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