

Carbonic acid, 2,2,2-trichloroethyl 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C11H11Cl3O3/c1-7-3-8(2)5-9(4-7)17-10(15)16-6-11(12,13)14/h3-5H,6H2,1-2H
InchiKey:	FULSZXNBYPXZFY-UHFFFAOYSA-N
Formula:	C11H11Cl3O3
SMILES:	Cc1cc(C)cc(OC(=O)OCC(Cl)(Cl)Cl)c1
Mol. weight [g/mol]:	297.56

Physical Properties

Property code	Value	Unit	Source
gf	-236.98	kJ/mol	Joback Method
hf	-489.77	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.189		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1836.00		NIST Webbook
tb	695.49	K	Joback Method
tc	927.08	K	Joback Method
tf	451.76	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.26	J/molxK	695.49	Joback Method
cpg	495.67	J/molxK	888.49	Joback Method
cpg	487.66	J/molxK	849.89	Joback Method
cpg	478.83	J/molxK	811.29	Joback Method
cpg	469.18	J/molxK	772.69	Joback Method
cpg	458.66	J/molxK	734.09	Joback Method
cpg	502.90	J/molxK	927.08	Joback Method
dvisc	0.0001068	Paxs	695.49	Joback Method
dvisc	0.0001338	Paxs	654.87	Joback Method

dvisc	0.0001726	Paxs	614.25	Joback Method
dvisc	0.0002308	Paxs	573.62	Joback Method
dvisc	0.0003227	Paxs	533.00	Joback Method
dvisc	0.0004768	Paxs	492.38	Joback Method
dvisc	0.0007557	Paxs	451.76	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=U357901&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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