Cyclopropanecarboxylic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C6H7Cl3O2/c7-6(8,9)3-11-5(10)4-1-2-4/h4H,1-3H2
InchiKey: KZZRCPHACUAIRF-UHFFFAOYSA-N
Formula: C6H7Cl3O2
SMILES: O=C(OCC(Cl)(Cl)Cl)C1CC1
Mol. weight [g/mol]: 217.48

Physical Properties

Property code	Value	Unit	Source
gf	-206.48	kJ/mol	Joback Method
hf	-395.14	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.310		Crippen Method
mcvol	128.700	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
tb	528.77	K	Joback Method
tc	752.92	K	Joback Method
tf	339.66	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.24	J/mol×K	528.77	Joback Method
cpg	270.30	J/mol×K	566.13	Joback Method
cpg	279.53	J/mol×K	603.49	Joback Method
cpg	287.99	J/mol×K	640.85	Joback Method
cpg	295.76	J/mol×K	678.20	Joback Method
cpg	302.88	J/mol×K	715.56	Joback Method
cpg	309.42	J/mol×K	752.92	Joback Method
dvisc	0.0028209	Pa×s	339.66	Joback Method

dvisc	0.0019473	Pa×s	371.18	Joback Method
dvisc	0.0014246	Pa×s	402.70	Joback Method
dvisc	0.0010906	Pa×s	434.22	Joback Method
dvisc	0.0008656	Pa×s	465.73	Joback Method
dvisc	0.0007075	Pa×s	497.25	Joback Method
dvisc	0.0005923	Pa×s	528.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354659&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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