Carbonic acid, 2,2,2-trichloroethyl 4-methoxyphenyl ester

Inchi: InChI=1S/C10H9Cl3O4/c1-15-7-2-4-8(5-3-7)17-9(14)16-6-10(11,12)13/h2-5H,6H2,1H3
InchiKey: QYIOUVUYTVIJTD-UHFFFAOYSA-N
Formula: C10H9Cl3O4
SMILES: COc1ccc(OC(=O)OCC(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 299.54

Physical Properties

Property code	Value	Unit	Source
gf	-340.77	kJ/mol	Joback Method
hf	-589.88	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.581		Crippen Method
mcvol	183.900	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	690.05	K	Joback Method
tc	922.00	K	Joback Method
tf	450.20	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.67	J/mol×K	690.05	Joback Method
cpg	433.36	J/mol×K	728.71	Joback Method
cpg	443.17	J/mol×K	767.37	Joback Method
cpg	452.12	J/mol×K	806.03	Joback Method
cpg	460.22	J/mol×K	844.69	Joback Method
cpg	467.49	J/mol×K	883.35	Joback Method
cpg	473.94	J/mol×K	922.00	Joback Method
dvisc	0.0006982	Pa×s	450.20	Joback Method

dvisc	0.0004359	Pa×s	490.18	Joback Method
dvisc	0.0002921	Pa×s	530.15	Joback Method
dvisc	0.0002071	Pa×s	570.12	Joback Method
dvisc	0.0001536	Pa×s	610.10	Joback Method
dvisc	0.0001182	Pa×s	650.08	Joback Method
dvisc	0.0000937	Pa×s	690.05	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=U357902&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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