Salicylic acid, 2,2,2-trichloroethyl carbonate

Inchi: InChI=1S/C10H7Cl3O5/c11-10(12,13)5-17-9(16)18-7-4-2-1-3-6(7)8(14)15/h1-4H,5H2,(H,
InchiKey: CMBKWDKPZGGVDA-UHFFFAOYSA-N
Formula: C10H7Cl3O5
SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccccc1C(=O)O
Mol. weight [g/mol]: 313.52
CAS: 20704-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-501.51	kJ/mol	Joback Method
hf	-722.47	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.270		Crippen Method
mcvol	185.470	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	813.68	K	Joback Method
tc	1037.46	K	Joback Method
tf	538.72	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.93	J/mol×K	813.68	Joback Method
cpg	473.68	J/mol×K	1000.17	Joback Method
cpg	469.46	J/mol×K	962.87	Joback Method
cpg	464.61	J/mol×K	925.57	Joback Method
cpg	459.09	J/mol×K	888.27	Joback Method
cpg	452.87	J/mol×K	850.98	Joback Method
cpg	477.28	J/mol×K	1037.46	Joback Method
dvisc	0.0000196	Pa×s	813.68	Joback Method
dvisc	0.0000272	Pa×s	767.85	Joback Method

dvisc	0.0000393	Pa×s	722.03	Joback Method
dvisc	0.0000596	Pa×s	676.20	Joback Method
dvisc	0.0000961	Pa×s	630.37	Joback Method
dvisc	0.0001671	Pa×s	584.55	Joback Method
dvisc	0.0003190	Pa×s	538.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20704998&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume