Trichloroacetic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C8H3Cl5O2/c9-5-2-1-4(3-6(5)10)15-7(14)8(11,12)13/h1-3H
InchiKey: HDGSKVNDSCZMPE-UHFFFAOYSA-N
Formula: C8H3Cl5O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-181.10	kJ/mol	Joback Method
hf	-327.11	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	66.79	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.269		Crippen Method
mcvol	168.460	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
tb	679.29	K	Joback Method
tc	935.40	K	Joback Method
tf	455.56	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.65	J/mol×K	679.29	Joback Method
cpg	327.75	J/mol×K	721.97	Joback Method
cpg	334.09	J/mol×K	764.66	Joback Method
cpg	339.73	J/mol×K	807.34	Joback Method
cpg	344.71	J/mol×K	850.03	Joback Method
cpg	349.09	J/mol×K	892.71	Joback Method
cpg	352.92	J/mol×K	935.40	Joback Method
dvisc	0.0009686	Pa×s	455.56	Joback Method

dvisc	0.0006437	Pa×s	492.85	Joback Method
dvisc	0.0004531	Pa×s	530.14	Joback Method
dvisc	0.0003340	Pa×s	567.42	Joback Method
dvisc	0.0002557	Pa×s	604.71	Joback Method
dvisc	0.0002019	Pa×s	642.00	Joback Method
dvisc	0.0001636	Pa×s	679.29	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=U307723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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