4-Penten-1-ol, trichloroacetate

Inchi: InChI=1S/C7H9Cl3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h2H,1,3-5H2
InchiKey: WMVZSMAZWDFZPH-UHFFFAOYSA-N
Formula: C7H9Cl3O2
SMILES: C=CCCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 231.50

Physical Properties

Property code	Value	Unit	Source
gf	-170.97	kJ/mol	Joback Method
hf	-363.15	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	51.52	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.866		Crippen Method
mcvol	149.350	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1228.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	541.59	K	Joback Method
tc	750.57	K	Joback Method
tf	331.23	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.82	J/mol×K	541.59	Joback Method
cpg	309.59	J/mol×K	576.42	Joback Method
cpg	318.70	J/mol×K	611.25	Joback Method
cpg	327.20	J/mol×K	646.08	Joback Method
cpg	335.11	J/mol×K	680.91	Joback Method
cpg	342.47	J/mol×K	715.74	Joback Method
cpg	349.30	J/mol×K	750.57	Joback Method
dvisc	0.0027774	Pa×s	331.23	Joback Method

dvisc	0.0015461	Pa×s	366.29	Joback Method
dvisc	0.0009534	Pa×s	401.35	Joback Method
dvisc	0.0006354	Pa×s	436.41	Joback Method
dvisc	0.0004498	Pa×s	471.47	Joback Method
dvisc	0.0003340	Pa×s	506.53	Joback Method
dvisc	0.0002578	Pa×s	541.59	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=R26514&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume