Trichloroacetic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C5H4Cl4O2/c6-2-1-3-11-4(10)5(7,8)9/h1-2H,3H2/b2-1+
InchiKey: KPJDOQORQYKCEB-OWOJBTEDSA-N
Formula: C5H4Cl4O2
SMILES: O=C(OCC=CCl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 237.90

Physical Properties

Property code	Value	Unit	Source
gf	-207.36	kJ/mol	Joback Method
hf	-345.82	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.652		Crippen Method
mcvol	133.410	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
tb	540.74	K	Joback Method
tc	766.95	K	Joback Method
tf	335.29	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.10	J/mol×K	540.74	Joback Method
cpg	242.96	J/mol×K	578.44	Joback Method
cpg	249.21	J/mol×K	616.14	Joback Method
cpg	254.91	J/mol×K	653.85	Joback Method
cpg	260.08	J/mol×K	691.55	Joback Method
cpg	264.79	J/mol×K	729.25	Joback Method
cpg	269.06	J/mol×K	766.95	Joback Method
dvisc	0.0025305	Pa×s	335.29	Joback Method

dvisc	0.0014354	Pa×s	369.53	Joback Method
dvisc	0.0008964	Pa×s	403.77	Joback Method
dvisc	0.0006025	Pa×s	438.01	Joback Method
dvisc	0.0004290	Pa×s	472.26	Joback Method
dvisc	0.0003199	Pa×s	506.50	Joback Method
dvisc	0.0002475	Pa×s	540.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299263&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume