Trichloroacetic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C7H9Cl3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h3H,4H2,1-2H3
InchiKey: NYRNTCPRCWEVKU-UHFFFAOYSA-N
Formula: C7H9Cl3O2
SMILES: CC(C)=CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 231.50

Physical Properties

Property code	Value	Unit	Source
gf	-187.14	kJ/mol	Joback Method
hf	-381.15	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.866		Crippen Method
mcvol	149.350	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1259.00		NIST Webbook
tb	548.95	K	Joback Method
tc	766.89	K	Joback Method
tf	313.95	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.20	J/mol×K	548.95	Joback Method
cpg	309.18	J/mol×K	585.27	Joback Method
cpg	318.45	J/mol×K	621.60	Joback Method
cpg	327.05	J/mol×K	657.92	Joback Method
cpg	335.02	J/mol×K	694.25	Joback Method
cpg	342.40	J/mol×K	730.57	Joback Method
cpg	349.25	J/mol×K	766.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299255&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
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