2-Propynyl trichloroacetate

Other names: 2-Propyn-1-ol, trichloroacetate
Inchi: InChI=1S/C5H3Cl3O2/c1-2-3-10-4(9)5(6,7)8/h1H,3H2
InchiKey: PGSHGNZXQJZXFA-UHFFFAOYSA-N
Formula: C5H3Cl3O2
SMILES: C#CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 201.44
CAS: 51698-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-52.58	kJ/mol	Joback Method
hf	-155.40	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.533		Crippen Method
mcvol	116.870	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
tb	489.27	K	Joback Method
tc	716.43	K	Joback Method
tf	357.42	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.16	J/mol×K	489.27	Joback Method
cpg	209.43	J/mol×K	527.13	Joback Method
cpg	215.17	J/mol×K	564.99	Joback Method
cpg	220.40	J/mol×K	602.85	Joback Method

cpg	225.17	J/mol×K	640.71	Joback Method
cpg	229.50	J/mol×K	678.57	Joback Method
cpg	233.43	J/mol×K	716.43	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=C51698772&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
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