Trichloroacetic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C7H5Cl3O2/c1-2-3-4-5-12-6(11)7(8,9)10/h1,3-4H,5H2
InchiKey: GRCGKUPJKHXUAF-UHFFFAOYSA-N
Formula: C7H5Cl3O2
SMILES: C#CC=CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 227.47

Physical Properties

Property code	Value	Unit	Source
gf	44.48	kJ/mol	Joback Method
hf	-79.46	kJ/mol	Joback Method
hfus	25.03	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.089		Crippen Method
mcvol	140.750	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
tb	539.19	K	Joback Method
tc	769.02	K	Joback Method
tf	374.88	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.71	J/mol×K	539.19	Joback Method
cpg	271.70	J/mol×K	577.50	Joback Method
cpg	278.99	J/mol×K	615.80	Joback Method
cpg	285.63	J/mol×K	654.11	Joback Method
cpg	291.68	J/mol×K	692.41	Joback Method
cpg	297.21	J/mol×K	730.72	Joback Method
cpg	302.25	J/mol×K	769.02	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=U299256&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume