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

Inchi: InChI=1S/C7H6Cl2O2/c1-2-3-4-5-11-7(10)6(8)9/h1,3-4,6H,5H2
InchiKey: NNFFABBXUJXUSY-UHFFFAOYSA-N
Formula: C7H6Cl2O2
SMILES: C#CC=CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 193.03

Physical Properties

Property code	Value	Unit	Source
gf	51.13	kJ/mol	Joback Method
hf	-60.25	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.523		Crippen Method
mcvol	128.510	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1184.00		NIST Webbook
tb	504.55	K	Joback Method
tc	720.18	K	Joback Method
tf	327.54	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.46	J/mol×K	504.55	Joback Method
cpg	247.77	J/mol×K	540.49	Joback Method
cpg	255.57	J/mol×K	576.43	Joback Method
cpg	262.86	J/mol×K	612.36	Joback Method
cpg	269.68	J/mol×K	648.30	Joback Method
cpg	276.06	J/mol×K	684.24	Joback Method
cpg	282.01	J/mol×K	720.18	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=U299431&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