Dichloroacetic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C8H10Cl2O2/c1-3-5-6(4-2)12-8(11)7(9)10/h6-7H,4H2,1-2H3
InchiKey: HNJCYURZVMLJAK-UHFFFAOYSA-N
Formula: C8H10Cl2O2
SMILES: CC#CC(CC)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 209.07

Physical Properties

Property code	Value	Unit	Source
gf	-43.38	kJ/mol	Joback Method
hf	-222.99	kJ/mol	Joback Method
hfus	23.73	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.135		Crippen Method
mcvol	146.900	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	541.71	K	Joback Method
tc	760.18	K	Joback Method
tf	388.02	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.53	J/mol×K	541.71	Joback Method
cpg	309.39	J/mol×K	578.12	Joback Method
cpg	319.70	J/mol×K	614.53	Joback Method
cpg	329.45	J/mol×K	650.95	Joback Method
cpg	338.67	J/mol×K	687.36	Joback Method
cpg	347.34	J/mol×K	723.77	Joback Method
cpg	355.49	J/mol×K	760.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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