Dichloroacetic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C13H18Cl2O2/c1-5-6-10(4)11(8-7-9(2)3)17-13(16)12(14)15/h10-12H,2,5-6H2,

InchiKey: WQHIJAZVGMYLTQ-UHFFFAOYSA-N

Formula: C13H18Cl2O2

SMILES: C=C(C)C#CC(OC(=O)C(Cl)Cl)C(C)CCC

Mol. weight [g/mol]: 277.19

Physical Properties

Property code	Value	Unit	Source
gf	75.57	kJ/mol	Joback Method
hf	-215.83	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	62.86	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.718		Crippen Method
mcvol	213.050	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	652.23	K	Joback Method
tc	864.90	K	Joback Method
tf	413.65	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.35	J/mol×K	652.23	Joback Method
cpg	530.11	J/mol×K	687.68	Joback Method
cpg	544.00	J/mol×K	723.12	Joback Method
cpg	557.07	J/mol×K	758.57	Joback Method
cpg	569.32	J/mol×K	794.01	Joback Method
cpg	580.79	J/mol×K	829.46	Joback Method
cpg	591.49	J/mol×K	864.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299435&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