Dichloroacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl

Inchi: InChI=1S/C12H16Cl2O2/c1-8(2)5-6-10(7-9(3)4)16-12(15)11(13)14/h9-11H,1,7H2,2-4H3

InchiKey: VSXCBHKTNKYJJP-UHFFFAOYSA-N

Formula: C12H16Cl2O2

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

Mol. weight [g/mol]: 263.16

Physical Properties

Property code	Value	Unit	Source
gf	67.15	kJ/mol	Joback Method
hf	-195.19	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.328		Crippen Method
mcvol	198.960	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1482.00		NIST Webbook
tb	629.35	K	Joback Method
tc	845.58	K	Joback Method
tf	402.38	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.05	J/mol×K	629.35	Joback Method
cpg	479.20	J/mol×K	665.39	Joback Method
cpg	492.53	J/mol×K	701.43	Joback Method
cpg	505.05	J/mol×K	737.46	Joback Method
cpg	516.79	J/mol×K	773.50	Joback Method
cpg	527.78	J/mol×K	809.54	Joback Method
cpg	538.03	J/mol×K	845.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299434&Units=SI

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