Dichloroacetic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C11H16Cl2O2/c1-4-5-6-9(7-8(2)3)15-11(14)10(12)13/h8-10H,4,7H2,1-3H3
InchiKey: AHCSRIQXLAZANZ-UHFFFAOYSA-N
Formula: C11H16Cl2O2
SMILES: CCC#CC(CC(C)C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 251.15

Physical Properties

Property code	Value	Unit	Source
gf	-20.56	kJ/mol	Joback Method
hf	-290.19	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.161		Crippen Method
mcvol	189.170	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	1431.00		NIST Webbook
rinpol	1431.00		NIST Webbook
tb	609.91	K	Joback Method
tc	821.92	K	Joback Method
tf	406.83	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.53	J/mol×K	609.91	Joback Method
cpg	451.45	J/mol×K	645.24	Joback Method
cpg	464.60	J/mol×K	680.58	Joback Method
cpg	477.01	J/mol×K	715.91	Joback Method
cpg	488.69	J/mol×K	751.25	Joback Method
cpg	499.66	J/mol×K	786.58	Joback Method
cpg	509.91	J/mol×K	821.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299433&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