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

Inchi: InChI=1S/C13H17Cl3O2/c1-5-6-10(4)11(8-7-9(2)3)18-12(17)13(14,15)16/h10-11H,2,5-6H

InchiKey: QUQXVSNIXBWVAX-UHFFFAOYSA-N

Formula: C13H17Cl3O2

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

Mol. weight [g/mol]: 311.63

Physical Properties

Property code	Value	Unit	Source
gf	68.92	kJ/mol	Joback Method
hf	-235.04	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	66.33	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.284		Crippen Method
mcvol	225.290	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	686.87	K	Joback Method
tc	910.36	K	Joback Method
tf	460.99	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.12	J/mol×K	686.87	Joback Method
cpg	558.03	J/mol×K	724.12	Joback Method
cpg	570.99	J/mol×K	761.37	Joback Method
cpg	583.05	J/mol×K	798.61	Joback Method
cpg	594.27	J/mol×K	835.86	Joback Method
cpg	604.69	J/mol×K	873.11	Joback Method
cpg	614.37	J/mol×K	910.36	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=U299260&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