Trichloroacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C12H15Cl3O2/c1-8(2)5-6-10(7-9(3)4)17-11(16)12(13,14)15/h9-10H,1,7H2,2-4

InchiKey: XXRBSODQKFUODU-UHFFFAOYSA-N

Formula: C12H15Cl3O2

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

Mol. weight [g/mol]: 297.61

Physical Properties

Property code	Value	Unit	Source
gf	60.50	kJ/mol	Joback Method
hf	-214.40	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	64.11	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.894		Crippen Method
mcvol	211.200	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1545.00		NIST Webbook
tb	663.99	K	Joback Method
tc	891.60	K	Joback Method
tf	449.72	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.40	J/mol×K	663.99	Joback Method
cpg	506.77	J/mol×K	701.93	Joback Method
cpg	519.21	J/mol×K	739.86	Joback Method
cpg	530.75	J/mol×K	777.80	Joback Method
cpg	541.46	J/mol×K	815.73	Joback Method
cpg	551.40	J/mol×K	853.67	Joback Method
cpg	560.60	J/mol×K	891.60	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=U299259&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