Trichloroacetic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C8H9Cl3O2/c1-3-5-6(4-2)13-7(12)8(9,10)11/h6H,4H2,1-2H3
InchiKey: ALHKHMGMXWSIDK-UHFFFAOYSA-N
Formula: C8H9Cl3O2
SMILES: CC#CC(CC)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 243.51

Physical Properties

Property code	Value	Unit	Source
gf	-50.03	kJ/mol	Joback Method
hf	-242.20	kJ/mol	Joback Method
hfus	24.04	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.702		Crippen Method
mcvol	159.140	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1317.00		NIST Webbook
tb	576.35	K	Joback Method
tc	808.21	K	Joback Method
tf	435.36	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.80	J/mol×K	576.35	Joback Method
cpg	335.29	J/mol×K	614.99	Joback Method
cpg	345.05	J/mol×K	653.64	Joback Method
cpg	354.11	J/mol×K	692.28	Joback Method
cpg	362.51	J/mol×K	730.92	Joback Method
cpg	370.27	J/mol×K	769.56	Joback Method
cpg	377.43	J/mol×K	808.21	Joback Method

Sources

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=U299257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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