Trichloroacetic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C15H23Cl3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-14(19)15(16,17)18/h2-10,13

InchiKey: IKJIABATPGGYLS-UHFFFAOYSA-N

Formula: C15H23Cl3O2

SMILES: CCCCCCCCCCC#CCOC(=O)C(Cl)(Cl)Cl

Mol. weight [g/mol]: 341.70

Physical Properties

Property code	Value	Unit	Source
gf	11.35	kJ/mol	Joback Method
hf	-381.40	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	72.15	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.434		Crippen Method
mcvol	257.770	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2084.00		NIST Webbook
tb	736.95	K	Joback Method
tc	940.54	K	Joback Method
tf	529.25	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.25	J/mol×K	736.95	Joback Method
cpg	687.91	J/mol×K	770.88	Joback Method
cpg	701.68	J/mol×K	804.81	Joback Method
cpg	714.61	J/mol×K	838.75	Joback Method
cpg	726.75	J/mol×K	872.68	Joback Method
cpg	738.12	J/mol×K	906.61	Joback Method
cpg	748.78	J/mol×K	940.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299262&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

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