Dichloroacetic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C15H24Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-15(18)14(16)17/h14H,2-10,1
InchiKey: DVLQUHLPIXUEAP-UHFFFAOYSA-N
Formula: C15H24Cl2O2
SMILES: CCCCCCCCCCC#CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 307.26

Physical Properties

Property code	Value	Unit	Source
gf	18.00	kJ/mol	Joback Method
hf	-362.19	kJ/mol	Joback Method
hfus	45.39	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.867		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	702.31	K	Joback Method
tc	896.67	K	Joback Method
tf	481.91	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.28	J/mol×K	702.31	Joback Method
cpg	658.80	J/mol×K	734.70	Joback Method
cpg	673.50	J/mol×K	767.10	Joback Method
cpg	687.39	J/mol×K	799.49	Joback Method
cpg	700.50	J/mol×K	831.88	Joback Method
cpg	712.84	J/mol×K	864.28	Joback Method
cpg	724.43	J/mol×K	896.67	Joback Method

Sources

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=U299437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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