3-Chloropropionic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C16H27ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-19-16(18)13-14-17/h2-10,13-15H
InchiKey: FWHBIDZGLNVDFD-UHFFFAOYSA-N
Formula: C16H27ClO2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCl
Mol. weight [g/mol]: 286.84

Physical Properties

Property code	Value	Unit	Source
gf	40.79	kJ/mol	Joback Method
hf	-361.81	kJ/mol	Joback Method
hfus	47.30	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.693		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	688.20	K	Joback Method
tc	874.33	K	Joback Method
tf	478.26	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.29	J/mol×K	688.20	Joback Method
cpg	683.89	J/mol×K	719.22	Joback Method
cpg	699.68	J/mol×K	750.24	Joback Method
cpg	714.68	J/mol×K	781.26	Joback Method
cpg	728.90	J/mol×K	812.29	Joback Method
cpg	742.36	J/mol×K	843.31	Joback Method
cpg	755.08	J/mol×K	874.33	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=U299220&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