Succinic acid, but-3-yn-2-yl 10-chlorodecyl ester

Inchi: InChI=1S/C18H29ClO4/c1-3-16(2)23-18(21)13-12-17(20)22-15-11-9-7-5-4-6-8-10-14-19/

InchiKey: KSNSNAHDIPUFPX-UHFFFAOYSA-N

Formula: C18H29ClO4

SMILES: C#CC(C)OC(=O)CCC(=O)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 344.87

Physical Properties

Property code	Value	Unit	Source
gf	-158.46	kJ/mol	Joback Method
hf	-633.57	kJ/mol	Joback Method
hfus	51.60	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.234		Crippen Method
mcvol	283.000	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	790.93	K	Joback Method
tc	980.42	K	Joback Method
tf	498.83	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.21	J/mol×K	790.93	Joback Method
cpg	842.86	J/mol×K	822.51	Joback Method
cpg	857.57	J/mol×K	854.09	Joback Method
cpg	871.39	J/mol×K	885.67	Joback Method
cpg	884.32	J/mol×K	917.26	Joback Method
cpg	896.38	J/mol×K	948.84	Joback Method
cpg	907.60	J/mol×K	980.42	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=U390404&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