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

Inchi: InChI=1S/C19H31ClO4/c1-3-17(2)24-19(22)14-12-13-18(21)23-16-11-9-7-5-4-6-8-10-15-

InchiKey: XLATXYDPCOMELU-UHFFFAOYSA-N

Formula: C19H31ClO4

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

Mol. weight [g/mol]: 358.90

Physical Properties

Property code	Value	Unit	Source
gf	-150.04	kJ/mol	Joback Method
hf	-654.21	kJ/mol	Joback Method
hfus	54.19	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.624		Crippen Method
mcvol	297.090	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	813.81	K	Joback Method
tc	1004.50	K	Joback Method
tf	510.10	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.43	J/mol×K	813.81	Joback Method
cpg	901.42	J/mol×K	845.59	Joback Method
cpg	916.45	J/mol×K	877.37	Joback Method
cpg	930.52	J/mol×K	909.16	Joback Method
cpg	943.67	J/mol×K	940.94	Joback Method
cpg	955.92	J/mol×K	972.72	Joback Method
cpg	967.28	J/mol×K	1004.50	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=U392453&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