Succinic acid, hex-4-yn-3-yl 10-chlorodecyl ester

Inchi: InChI=1S/C20H33ClO4/c1-3-13-18(4-2)25-20(23)15-14-19(22)24-17-12-10-8-6-5-7-9-11-

InchiKey: LJBRGRWKKUFSLJ-UHFFFAOYSA-N

Formula: C20H33ClO4

SMILES: CC#CC(CC)OC(=O)CCC(=O)OCCCCCCCCCCCl

Mol. weight [g/mol]: 372.93

Physical Properties

Property code	Value	Unit	Source
gf	-161.89	kJ/mol	Joback Method
hf	-694.45	kJ/mol	Joback Method
hfus	56.93	kJ/mol	Joback Method
hvap	84.58	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.014		Crippen Method
mcvol	311.180	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	855.57	K	Joback Method
tc	1053.44	K	Joback Method
tf	580.50	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.00	J/mol×K	855.57	Joback Method
cpg	966.42	J/mol×K	888.55	Joback Method
cpg	981.73	J/mol×K	921.53	Joback Method
cpg	995.97	J/mol×K	954.50	Joback Method
cpg	1009.15	J/mol×K	987.48	Joback Method
cpg	1021.28	J/mol×K	1020.46	Joback Method
cpg	1032.38	J/mol×K	1053.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390409&Units=SI

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