Succinic acid, hex-4-yn-3-yl 2-chloro-4-methylphenyl ester

Inchi: InChI=1S/C17H19ClO4/c1-4-6-13(5-2)21-16(19)9-10-17(20)22-15-8-7-12(3)11-14(15)18/

InchiKey: NJXCDZVKULALPB-UHFFFAOYSA-N

Formula: C17H19ClO4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(C)cc1Cl

Mol. weight [g/mol]: 322.78

Physical Properties

Property code	Value	Unit	Source
gf	-94.00	kJ/mol	Joback Method
hf	-418.94	kJ/mol	Joback Method
hfus	42.42	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.679		Crippen Method
mcvol	245.150	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	823.57	K	Joback Method
tc	1047.79	K	Joback Method
tf	598.15	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.69	J/mol×K	823.57	Joback Method
cpg	693.37	J/mol×K	860.94	Joback Method
cpg	705.93	J/mol×K	898.31	Joback Method
cpg	717.38	J/mol×K	935.68	Joback Method
cpg	727.72	J/mol×K	973.05	Joback Method
cpg	736.96	J/mol×K	1010.42	Joback Method
cpg	745.12	J/mol×K	1047.79	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=U390216&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