Succinic acid, hex-4-yn-3-yl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C16H16Cl2O4/c1-3-5-13(4-2)21-15(19)6-7-16(20)22-14-9-11(17)8-12(18)10-14

InchiKey: DPYAWNKANNYCOB-UHFFFAOYSA-N

Formula: C16H16Cl2O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 343.20

Physical Properties

Property code	Value	Unit	Source
gf	-114.35	kJ/mol	Joback Method
hf	-414.04	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.024		Crippen Method
mcvol	243.300	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	838.12	K	Joback Method
tc	1068.04	K	Joback Method
tf	616.80	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.19	J/mol×K	838.12	Joback Method
cpg	659.36	J/mol×K	876.44	Joback Method
cpg	670.44	J/mol×K	914.76	Joback Method
cpg	680.42	J/mol×K	953.08	Joback Method
cpg	689.32	J/mol×K	991.40	Joback Method
cpg	697.15	J/mol×K	1029.72	Joback Method
cpg	703.91	J/mol×K	1068.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390149&Units=SI
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

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