Succinic acid, hex-4-yn-3-yl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H15Cl3O4/c1-3-5-10(4-2)22-15(20)6-7-16(21)23-14-9-12(18)11(17)8-13(14

InchiKey: GGECSLSXXVKVIR-UHFFFAOYSA-N

Formula: C16H15Cl3O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 377.65

Physical Properties

Property code	Value	Unit	Source
gf	-135.91	kJ/mol	Joback Method
hf	-441.25	kJ/mol	Joback Method
hfus	47.83	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.678		Crippen Method
mcvol	255.540	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	880.53	K	Joback Method
tc	1114.03	K	Joback Method
tf	659.24	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.69	J/mol×K	880.53	Joback Method
cpg	677.52	J/mol×K	919.45	Joback Method
cpg	687.24	J/mol×K	958.36	Joback Method
cpg	695.84	J/mol×K	997.28	Joback Method
cpg	703.34	J/mol×K	1036.20	Joback Method
cpg	709.73	J/mol×K	1075.11	Joback Method
cpg	715.01	J/mol×K	1114.03	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=U389965&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