Succinic acid, hex-4-yn-3-yl pentachlorophenyl ester

Inchi: InChI=1S/C16H13Cl5O4/c1-3-5-8(4-2)24-9(22)6-7-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: GHGGYBBXDSIBDS-UHFFFAOYSA-N

Formula: C16H13Cl5O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 446.54

Physical Properties

Property code	Value	Unit	Source
gf	-179.03	kJ/mol	Joback Method
hf	-495.67	kJ/mol	Joback Method
hfus	55.45	kJ/mol	Joback Method
hvap	98.80	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	5.984		Crippen Method
mcvol	280.020	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	965.35	K	Joback Method
tc	1206.56	K	Joback Method
tf	744.12	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.82	J/mol×K	965.35	Joback Method
cpg	707.91	J/mol×K	1005.55	Joback Method
cpg	714.81	J/mol×K	1045.75	Joback Method
cpg	720.51	J/mol×K	1085.95	Joback Method
cpg	725.00	J/mol×K	1126.15	Joback Method
cpg	728.27	J/mol×K	1166.35	Joback Method
cpg	730.31	J/mol×K	1206.56	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=U390048&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