Succinic acid, tridec-2-yn-1-yl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C23H29Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-29-22(27)13-14-23(28)30-21-17

InchiKey: XGAHYYQIRWSVGI-UHFFFAOYSA-N

Formula: C23H29Cl3O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 475.83

Physical Properties

Property code	Value	Unit	Source
gf	-74.53	kJ/mol	Joback Method
hf	-580.45	kJ/mol	Joback Method
hfus	69.49	kJ/mol	Joback Method
hvap	104.67	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	7.410		Crippen Method
mcvol	354.170	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	3238.00		NIST Webbook
rinpol	3238.00		NIST Webbook
tb	1041.13	K	Joback Method
tc	1275.45	K	Joback Method
tf	753.13	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1070.99	J/mol×K	1041.13	Joback Method
cpg	1082.76	J/mol×K	1080.18	Joback Method
cpg	1093.10	J/mol×K	1119.24	Joback Method
cpg	1102.04	J/mol×K	1158.29	Joback Method
cpg	1109.60	J/mol×K	1197.35	Joback Method
cpg	1115.83	J/mol×K	1236.40	Joback Method
cpg	1120.76	J/mol×K	1275.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389977&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

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