Succinic acid, tridec-2-yn-1-yl 3-chlorophenyl ester

Inchi: InChI=1S/C23H31ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-18-27-22(25)16-17-23(26)28-21-15-

InchiKey: KAMXRXATTZHJKL-UHFFFAOYSA-N

Formula: C23H31ClO4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 406.94

Physical Properties

Property code	Value	Unit	Source
gf	-31.41	kJ/mol	Joback Method
hf	-526.03	kJ/mol	Joback Method
hfus	61.87	kJ/mol	Joback Method
hvap	94.58	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.103		Crippen Method
mcvol	329.690	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	956.31	K	Joback Method
tc	1175.32	K	Joback Method
tf	668.25	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.24	J/mol×K	956.31	Joback Method
cpg	1043.83	J/mol×K	992.81	Joback Method
cpg	1057.10	J/mol×K	1029.31	Joback Method
cpg	1069.09	J/mol×K	1065.82	Joback Method
cpg	1079.85	J/mol×K	1102.32	Joback Method
cpg	1089.40	J/mol×K	1138.82	Joback Method
cpg	1097.78	J/mol×K	1175.32	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=U389860&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