Succinic acid, 2-chloro-6-fluorophenyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C22H28ClFO4/c1-2-3-4-5-6-7-8-9-10-11-17-27-20(25)15-16-21(26)28-22-18(23

InchiKey: MJWPPLIARDXYFO-UHFFFAOYSA-N

Formula: C22H28ClFO4

SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 410.91

Physical Properties

Property code	Value	Unit	Source
gf	-244.27	kJ/mol	Joback Method
hf	-712.97	kJ/mol	Joback Method
hfus	61.97	kJ/mol	Joback Method
hvap	92.20	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.852		Crippen Method
mcvol	317.370	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2891.00		NIST Webbook
tb	937.68	K	Joback Method
tc	1152.70	K	Joback Method
tf	670.09	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.40	J/mol×K	937.68	Joback Method
cpg	989.42	J/mol×K	973.52	Joback Method
cpg	1002.20	J/mol×K	1009.35	Joback Method
cpg	1013.74	J/mol×K	1045.19	Joback Method
cpg	1024.10	J/mol×K	1081.03	Joback Method
cpg	1033.28	J/mol×K	1116.86	Joback Method
cpg	1041.31	J/mol×K	1152.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391002&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