Succinic acid, tridec-2-yn-1-yl 2-fluorophenyl ester

Inchi: InChI=1S/C23H31FO4/c1-2-3-4-5-6-7-8-9-10-11-14-19-27-22(25)17-18-23(26)28-21-16-1

InchiKey: RFKLEPPJRQZUAC-UHFFFAOYSA-N

Formula: C23H31FO4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 390.49

Physical Properties

Property code	Value	Unit	Source
gf	-214.29	kJ/mol	Joback Method
hf	-706.40	kJ/mol	Joback Method
hfus	60.75	kJ/mol	Joback Method
hvap	89.38	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.589		Crippen Method
mcvol	319.220	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	918.15	K	Joback Method
tc	1128.33	K	Joback Method
tf	638.92	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.08	J/mol×K	918.15	Joback Method
cpg	1026.58	J/mol×K	953.18	Joback Method
cpg	1040.83	J/mol×K	988.21	Joback Method
cpg	1053.84	J/mol×K	1023.24	Joback Method
cpg	1065.66	J/mol×K	1058.27	Joback Method
cpg	1076.31	J/mol×K	1093.30	Joback Method
cpg	1085.82	J/mol×K	1128.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390318&Units=SI

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