Succinic acid, tridec-2-yn-1-yl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C24H30F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-31-21(29)16-17-22(30)32-20-15

InchiKey: GXFYXGQDTMHULL-UHFFFAOYSA-N

Formula: C24H30F4O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 458.49

Physical Properties

Property code	Value	Unit	Source
gf	-797.09	kJ/mol	Joback Method
hf	-1335.59	kJ/mol	Joback Method
hfus	64.78	kJ/mol	Joback Method
hvap	88.52	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.608		Crippen Method
mcvol	338.620	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	940.59	K	Joback Method
tc	1151.67	K	Joback Method
tf	666.90	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.02	J/mol×K	940.59	Joback Method
cpg	1106.98	J/mol×K	975.77	Joback Method
cpg	1120.72	J/mol×K	1010.95	Joback Method
cpg	1133.30	J/mol×K	1046.13	Joback Method
cpg	1144.76	J/mol×K	1081.31	Joback Method
cpg	1155.16	J/mol×K	1116.49	Joback Method
cpg	1164.55	J/mol×K	1151.67	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=U390794&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