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

Inchi: InChI=1S/C23H27F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-31-16(29)13-14-17(30)32-23-21
InchiKey: RLINMEXPRSBOCQ-UHFFFAOYSA-N
Formula: C23H27F5O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 462.45

Physical Properties

Property code	Value	Unit	Source
gf	-1032.05	kJ/mol	Joback Method
hf	-1536.72	kJ/mol	Joback Method
hfus	71.52	kJ/mol	Joback Method
hvap	88.76	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.145		Crippen Method
mcvol	326.300	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	935.15	K	Joback Method
tc	1145.13	K	Joback Method
tf	691.36	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.90	J/mol×K	935.15	Joback Method
cpg	1050.25	J/mol×K	970.15	Joback Method
cpg	1063.30	J/mol×K	1005.14	Joback Method
cpg	1075.07	J/mol×K	1040.14	Joback Method
cpg	1085.56	J/mol×K	1075.14	Joback Method
cpg	1094.78	J/mol×K	1110.14	Joback Method
cpg	1102.76	J/mol×K	1145.13	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=U390358&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