Succinic acid, hex-4-yn-3-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H15F3O4/c1-3-5-10(4-2)22-13(20)8-9-14(21)23-12-7-6-11(17)15(18)16(12

InchiKey: YDOCRBWULUAUSQ-UHFFFAOYSA-N

Formula: C16H15F3O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 328.28

Physical Properties

Property code	Value	Unit	Source
gf	-684.55	kJ/mol	Joback Method
hf	-982.36	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	73.10	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.135		Crippen Method
mcvol	224.130	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1951.00		NIST Webbook
tb	766.05	K	Joback Method
tc	968.48	K	Joback Method
tf	571.25	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.88	J/mol×K	766.05	Joback Method
cpg	634.70	J/mol×K	799.79	Joback Method
cpg	646.65	J/mol×K	833.53	Joback Method
cpg	657.72	J/mol×K	867.26	Joback Method
cpg	667.92	J/mol×K	901.00	Joback Method
cpg	677.25	J/mol×K	934.74	Joback Method
cpg	685.70	J/mol×K	968.48	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=U390760&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