Succinic acid, hept-2-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H21F3O4/c1-3-4-5-6-11(2)23-14(21)9-10-15(22)24-13-8-7-12(18)16(19)17

InchiKey: KSXDGIGTIXLFOS-UHFFFAOYSA-N

Formula: C17H21F3O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-878.93	kJ/mol	Joback Method
hf	-1275.30	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.301		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	779.93	K	Joback Method
tc	968.69	K	Joback Method
tf	476.42	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.20	J/mol×K	779.93	Joback Method
cpg	740.18	J/mol×K	811.39	Joback Method
cpg	753.27	J/mol×K	842.85	Joback Method
cpg	765.47	J/mol×K	874.31	Joback Method
cpg	776.80	J/mol×K	905.77	Joback Method
cpg	787.25	J/mol×K	937.23	Joback Method
cpg	796.83	J/mol×K	968.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390761&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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