Succinic acid, 1,1,1-trifluoroprop-2-yl oct-1-en-3-yl ester

Inchi: InChI=1S/C15H23F3O4/c1-4-6-7-8-12(5-2)22-14(20)10-9-13(19)21-11(3)15(16,17)18/h5

InchiKey: QNXBOKWZLWBLLM-UHFFFAOYSA-N

Formula: C15H23F3O4

SMILES: C=CC(CCCCC)OC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-891.05	kJ/mol	Joback Method
hf	-1324.74	kJ/mol	Joback Method
hfus	33.68	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.939		Crippen Method
mcvol	238.100	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
tb	685.56	K	Joback Method
tc	858.27	K	Joback Method
tf	375.56	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.39	J/mol×K	685.56	Joback Method
cpg	695.25	J/mol×K	714.34	Joback Method
cpg	709.31	J/mol×K	743.13	Joback Method
cpg	722.62	J/mol×K	771.91	Joback Method
cpg	735.18	J/mol×K	800.70	Joback Method
cpg	747.02	J/mol×K	829.48	Joback Method
cpg	758.16	J/mol×K	858.27	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=U391314&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