Succinic acid, 3-methylbut-2-en-1-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C15H15F3O4/c1-9(2)7-8-21-12(19)5-6-13(20)22-11-4-3-10(16)14(17)15(11)18

InchiKey: WWAAVPHVKMDEAJ-UHFFFAOYSA-N

Formula: C15H15F3O4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
gf	-821.66	kJ/mol	Joback Method
hf	-1121.31	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.299		Crippen Method
mcvol	214.340	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	738.65	K	Joback Method
tc	932.27	K	Joback Method
tf	449.84	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.69	J/mol×K	738.65	Joback Method
cpg	603.24	J/mol×K	770.92	Joback Method
cpg	615.02	J/mol×K	803.19	Joback Method
cpg	626.04	J/mol×K	835.46	Joback Method
cpg	636.32	J/mol×K	867.73	Joback Method
cpg	645.87	J/mol×K	900.00	Joback Method
cpg	654.70	J/mol×K	932.27	Joback Method

Sources

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=U390758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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