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

Inchi: InChI=1S/C15H17F3O4/c1-8(2)9(3)21-12(19)6-7-13(20)22-11-5-4-10(16)14(17)15(11)18

InchiKey: FSWPIRQTEYQCJC-UHFFFAOYSA-N

Formula: C15H17F3O4

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

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-898.21	kJ/mol	Joback Method
hf	-1239.30	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.377		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1799.00		NIST Webbook
rinpol	1799.00		NIST Webbook
tb	733.73	K	Joback Method
tc	924.83	K	Joback Method
tf	438.88	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.37	J/mol×K	733.73	Joback Method
cpg	629.73	J/mol×K	765.58	Joback Method
cpg	642.26	J/mol×K	797.43	Joback Method
cpg	653.98	J/mol×K	829.28	Joback Method
cpg	664.88	J/mol×K	861.13	Joback Method
cpg	674.96	J/mol×K	892.98	Joback Method
cpg	684.23	J/mol×K	924.83	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=U390756&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