Succinic acid, 1,1,1-trifluoroprop-2-yl 2,3-dimethylphenyl ester

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

InchiKey: MMVJTMMWXODNKR-UHFFFAOYSA-N

Formula: C15H17F3O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OC(C)C(F)(F)F)c1C

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-883.30	kJ/mol	Joback Method
hf	-1231.30	kJ/mol	Joback Method
hfus	31.75	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.483		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	725.96	K	Joback Method
tc	920.94	K	Joback Method
tf	443.78	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.18	J/mol×K	725.96	Joback Method
cpg	632.69	J/mol×K	758.46	Joback Method
cpg	645.31	J/mol×K	790.95	Joback Method
cpg	657.08	J/mol×K	823.45	Joback Method
cpg	668.00	J/mol×K	855.95	Joback Method
cpg	678.11	J/mol×K	888.45	Joback Method
cpg	687.41	J/mol×K	920.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390012&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