Succinic acid, ethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C12H11F3O4/c1-2-18-9(16)5-6-10(17)19-8-4-3-7(13)11(14)12(8)15/h3-4H,2,5-
InchiKey: QBPJDFUOJQHHCU-UHFFFAOYSA-N
Formula: C12H11F3O4
SMILES: CCOC(=O)CCC(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 276.21

Physical Properties

Property code	Value	Unit	Source
gf	-918.59	kJ/mol	Joback Method
hf	-1166.82	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.353		Crippen Method
mcvol	176.370	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	665.97	K	Joback Method
tc	855.23	K	Joback Method
tf	435.07	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.60	J/mol×K	665.97	Joback Method
cpg	469.97	J/mol×K	697.51	Joback Method
cpg	480.72	J/mol×K	729.06	Joback Method
cpg	490.85	J/mol×K	760.60	Joback Method
cpg	500.36	J/mol×K	792.14	Joback Method
cpg	509.24	J/mol×K	823.69	Joback Method
cpg	517.49	J/mol×K	855.23	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=U390775&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