Succinic acid, ethyl 2-fluorophenyl ester

Inchi: InChI=1S/C12H13FO4/c1-2-16-11(14)7-8-12(15)17-10-6-4-3-5-9(10)13/h3-6H,2,7-8H2,1
InchiKey: ZIYNLKGHTNDDTF-UHFFFAOYSA-N
Formula: C12H13FO4
SMILES: CCOC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 240.23

Physical Properties

Property code	Value	Unit	Source
gf	-509.71	kJ/mol	Joback Method
hf	-751.66	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	62.74	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.074		Crippen Method
mcvol	172.830	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	657.47	K	Joback Method
tc	860.46	K	Joback Method
tf	408.85	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.57	J/mol×K	657.47	Joback Method
cpg	457.30	J/mol×K	691.30	Joback Method
cpg	469.28	J/mol×K	725.13	Joback Method
cpg	480.50	J/mol×K	758.97	Joback Method
cpg	490.98	J/mol×K	792.80	Joback Method
cpg	500.72	J/mol×K	826.63	Joback Method
cpg	509.70	J/mol×K	860.46	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=U390321&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