Succinic acid, 3-methylbut-2-yl 3-fluorophenyl ester

Inchi: InChI=1S/C15H19FO4/c1-10(2)11(3)19-14(17)7-8-15(18)20-13-6-4-5-12(16)9-13/h4-6,9-

InchiKey: DETDABVVJFEESL-UHFFFAOYSA-N

Formula: C15H19FO4

SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 282.31

Physical Properties

Property code	Value	Unit	Source
gf	-489.33	kJ/mol	Joback Method
hf	-824.14	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.099		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	725.23	K	Joback Method
tc	927.82	K	Joback Method
tf	412.66	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.53	J/mol×K	725.23	Joback Method
cpg	617.19	J/mol×K	758.99	Joback Method
cpg	630.90	J/mol×K	792.76	Joback Method
cpg	643.67	J/mol×K	826.52	Joback Method
cpg	655.51	J/mol×K	860.29	Joback Method
cpg	666.43	J/mol×K	894.05	Joback Method
cpg	676.43	J/mol×K	927.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390326&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