Succinic acid, 3-methylbut-2-en-1-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C16H19FO5/c1-11(2)8-9-21-15(18)6-7-16(19)22-13-5-4-12(17)10-14(13)20-3/h

InchiKey: KDQKHJABYFIGLF-UHFFFAOYSA-N

Formula: C16H19FO5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 310.32

Physical Properties

Property code	Value	Unit	Source
gf	-518.99	kJ/mol	Joback Method
hf	-870.48	kJ/mol	Joback Method
hfus	39.19	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.029		Crippen Method
mcvol	230.760	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	780.43	K	Joback Method
tc	984.00	K	Joback Method
tf	469.64	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.49	J/mol×K	780.43	Joback Method
cpg	671.23	J/mol×K	814.36	Joback Method
cpg	684.04	J/mol×K	848.29	Joback Method
cpg	695.91	J/mol×K	882.21	Joback Method
cpg	706.84	J/mol×K	916.14	Joback Method
cpg	716.86	J/mol×K	950.07	Joback Method
cpg	725.96	J/mol×K	984.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390900&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