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

Inchi: InChI=1S/C16H21FO5/c1-10(2)11(3)21-15(18)7-8-16(19)22-13-6-5-12(17)9-14(13)20-4/h

InchiKey: LSBNCSPSPRUBHS-UHFFFAOYSA-N

Formula: C16H21FO5

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

Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-595.54	kJ/mol	Joback Method
hf	-988.47	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	73.94	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.108		Crippen Method
mcvol	235.060	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	775.51	K	Joback Method
tc	976.52	K	Joback Method
tf	458.68	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.18	J/mol×K	775.51	Joback Method
cpg	698.69	J/mol×K	809.01	Joback Method
cpg	712.18	J/mol×K	842.51	Joback Method
cpg	724.65	J/mol×K	876.02	Joback Method
cpg	736.10	J/mol×K	909.52	Joback Method
cpg	746.52	J/mol×K	943.02	Joback Method
cpg	755.91	J/mol×K	976.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390898&Units=SI

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