Succinic acid, hept-2-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25FO5/c1-4-5-6-7-13(2)23-17(20)10-11-18(21)24-15-9-8-14(19)12-16(15

InchiKey: GTVFJRZEAPMMNU-UHFFFAOYSA-N

Formula: C18H25FO5

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 340.39

Physical Properties

Property code	Value	Unit	Source
gf	-576.26	kJ/mol	Joback Method
hf	-1024.47	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	78.78	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.032		Crippen Method
mcvol	263.240	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	821.71	K	Joback Method
tc	1019.87	K	Joback Method
tf	496.22	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.23	J/mol×K	821.71	Joback Method
cpg	812.08	J/mol×K	854.74	Joback Method
cpg	825.85	J/mol×K	887.76	Joback Method
cpg	838.52	J/mol×K	920.79	Joback Method
cpg	850.12	J/mol×K	953.82	Joback Method
cpg	860.62	J/mol×K	986.85	Joback Method
cpg	870.04	J/mol×K	1019.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390903&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