Succinic acid, 2-fluorophenyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C18H21FO4/c1-13-6-2-3-7-14(13)12-22-17(20)10-11-18(21)23-16-9-5-4-8-15(1

InchiKey: ZYMAWRYJCPOTPT-UHFFFAOYSA-N

Formula: C18H21FO4

SMILES: CC1=C(COC(=O)CCC(=O)Oc2ccccc2F)CCCC1

Mol. weight [g/mol]: 320.36

Physical Properties

Property code	Value	Unit	Source
gf	-416.33	kJ/mol	Joback Method
hf	-766.00	kJ/mol	Joback Method
hfus	35.89	kJ/mol	Joback Method
hvap	78.45	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.945		Crippen Method
mcvol	242.210	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	828.09	K	Joback Method
tc	1047.04	K	Joback Method
tf	513.89	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.07	J/mol×K	828.09	Joback Method
cpg	745.01	J/mol×K	864.58	Joback Method
cpg	758.68	J/mol×K	901.07	Joback Method
cpg	771.10	J/mol×K	937.57	Joback Method
cpg	782.31	J/mol×K	974.06	Joback Method
cpg	792.31	J/mol×K	1010.55	Joback Method
cpg	801.14	J/mol×K	1047.04	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=U391418&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