Succinic acid, 2-fluorophenyl cyclopentyl ester

Inchi: InChI=1S/C15H17FO4/c16-12-7-3-4-8-13(12)20-15(18)10-9-14(17)19-11-5-1-2-6-11/h3-4

InchiKey: FSWMHJTYSAIZKC-UHFFFAOYSA-N

Formula: C15H17FO4

SMILES: O=C(CCC(=O)OC1CCCC1)Oc1ccccc1F

Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-447.90	kJ/mol	Joback Method
hf	-753.10	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	69.67	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.997		Crippen Method
mcvol	204.240	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	741.39	K	Joback Method
tc	959.68	K	Joback Method
tf	453.56	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.39	J/mol×K	741.39	Joback Method
cpg	606.88	J/mol×K	777.77	Joback Method
cpg	621.20	J/mol×K	814.15	Joback Method
cpg	634.38	J/mol×K	850.54	Joback Method
cpg	646.44	J/mol×K	886.92	Joback Method
cpg	657.40	J/mol×K	923.30	Joback Method
cpg	667.29	J/mol×K	959.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391375&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