Succinic acid, di(4-fluorobenzyl) ester

Inchi: InChI=1S/C18H16F2O4/c19-15-5-1-13(2-6-15)11-23-17(21)9-10-18(22)24-12-14-3-7-16(
InchiKey: ILEFIRBZNDGHFF-UHFFFAOYSA-N
Formula: C18H16F2O4
SMILES: O=C(CCC(=O)OCc1ccc(F)cc1)OCc1ccc(F)cc1
Mol. weight [g/mol]: 334.31

Physical Properties

Property code	Value	Unit	Source
gf	-551.22	kJ/mol	Joback Method
hf	-846.55	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.532		Crippen Method
mcvol	235.380	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	825.68	K	Joback Method
tc	1040.41	K	Joback Method
tf	516.00	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.99	J/mol×K	825.68	Joback Method
cpg	694.76	J/mol×K	861.47	Joback Method
cpg	706.42	J/mol×K	897.26	Joback Method
cpg	717.01	J/mol×K	933.04	Joback Method
cpg	726.55	J/mol×K	968.83	Joback Method
cpg	735.06	J/mol×K	1004.62	Joback Method
cpg	742.55	J/mol×K	1040.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381684&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