Succinic acid, 4-cyanophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H12FNO4/c18-13-2-1-3-15(10-13)23-17(21)9-8-16(20)22-14-6-4-12(11-19)
InchiKey: MWCYYVAWHOAGSB-UHFFFAOYSA-N
Formula: C17H12FNO4
SMILES: N#Cc1ccc(OC(=O)CCC(=O)Oc2cccc(F)c2)cc1
Mol. weight [g/mol]: 313.28

Physical Properties

Property code	Value	Unit	Source
gf	-231.65	kJ/mol	Joback Method
hf	-464.92	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	87.28	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	2.989		Crippen Method
mcvol	220.900	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2532.00		NIST Webbook
tb	905.61	K	Joback Method
tc	1140.82	K	Joback Method
tf	569.13	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.86	J/mol×K	905.61	Joback Method
cpg	640.38	J/mol×K	944.81	Joback Method
cpg	648.74	J/mol×K	984.01	Joback Method
cpg	655.99	J/mol×K	1023.22	Joback Method
cpg	662.12	J/mol×K	1062.42	Joback Method
cpg	667.18	J/mol×K	1101.62	Joback Method
cpg	671.18	J/mol×K	1140.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360705&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